

# Kernel Additive Principal Components

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## Abstract

Additive principal components (APCs for short) are a nonlinear generalization of linear principal components. We focus on smallest APCs to describe additive nonlinear constraints that are approximately satisfied by the data. Thus APCs fit data with implicit equations that treat the variables symmetrically, as opposed to regression analyses which fit data with explicit equations that treat the data asymmetrically by singling out a response variable. We propose a regularized data-analytic procedure for APC estimation using kernel methods. In contrast to existing approaches to APCs that are based on regularization through subspace restriction, kernel methods achieve regularization through shrinkage and therefore grant distinctive flexibility in APC estimation by allowing the use of infinite-dimensional functions spaces for searching APC transformation while retaining computational feasibility. To connect population APCs and kernelized finite-sample APCs, we study kernelized population APCs and their associated eigenproblems, which eventually lead to the establishment of consistency of the estimated APCs. Lastly, we discuss an iterative algorithm for computing kernelized finite-sample APCs.

**Keywords:** *Additive models, kernel methods, nonlinear multivariate analysis, principal components, reproducing kernel Hilbert space.*

## 1 Introduction

Principal component analysis (PCA) is a tool commonly used to reduce the dimensionality of data sets consisting of a large number of interrelated variables  $X_1, X_2, \dots, X_p$ . PCA amounts to finding linear functions of the variables,  $\sum a_j X_j$ , whose variances are maximal or, more generally, large and stationary under a unit norm constraint,  $\sum a_j^2 = 1$ . These linear combinations, called *largest linear principal components*, are thought to represent low-dimensional linear structure of the data. The reader is referred to Jolliffe (2002) for a comprehensive review of PCA.

One can similarly define the *smallest linear principal component* as linear functions of the variables whose variances are minimal or small and stationary subject to a unit norm constraint on the coefficients. If these variances are near zero,  $\text{Var}(\sum a_j X_j) \approx 0$ , the interpretation is that the data lie near the hyperplane defined by the linear constraint  $\sum a_j X_j = 0$  (assuming that the

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variables  $X_j$  are centered). Thus the purpose of performing PCA on the lower end of the principal components spectrum is quite different from that of performing it on the upper end: largest principal components are concerned with structure of *low dimension*, whereas smallest principal components are concerned with structure of *low codimension*.

Smallest additive principal components (“APCs” for short) are a nonlinear generalization of smallest linear principal components (“LPCs” for short), initially proposed in [Donnell et al. \(1994\)](#). The *smallest APC* is defined as an additive function of the variables,  $\sum \phi_j(X_j)$ , with smallest variance subject to a normalizing constraint  $\sum \|\phi_j(X_j)\|^2 = 1$ . The interpretation of a smallest APC is that the additive constraint represented by the implicit additive equation  $\sum \phi_j(X_j) = 0$  defines a nonlinear manifold that approximates the data. The focus of the current paper will be on smallest APCs, and we will therefore sometimes drop the adjective “smallest”. Smallest APCs can be motivated in several ways:

- APCs can be used as a generalized collinearity diagnostic for additive regression models. Just as approximate collinearities  $\sum \beta_j X_j \approx 0$  destabilize inference in linear regression, additive approximate “concurvities” ([Donnell et al., 1994](#)) of the form  $\sum \phi_j(X_j) \approx 0$  destabilize inference in additive regression. Such concurvities can be found by applying APC analysis to the predictors of an additive regression.
- APCs can also be used as a symmetric alternative to additive regression as well as to ACE regression ([Breiman and Friedman, 1985](#)) when it is not possible or not desirable to single out any one of the variables as a response. Additive implicit equations estimated with APCs will then freely identify the variables that have strong additive associations with each other.
- Even when there is a specific response variable of interest in the context of an additive regression, an APC analysis of all variables, predictors as well as response, can serve as an indicator of the strength of the regression, depending on whether the response variable has a strong presence in the smallest APC. If the response shows up only weakly, it follows that the predictors have stronger additive associations among each other than with the response.

Estimation of APCs and their transforms  $\phi_j(X_j)$  from finite data requires some form of regularization. There exist two broad classes of regularization in nonparametric function estimation, namely, subspace regularization and shrinkage regularization. Subspace regularization restricts the function estimates  $\hat{\phi}_j$  to finite-dimensional function spaces on  $X_j$ . Shrinkage regularization produces function estimates by adding a penalty to the goodness-of-fit measure in order to impose the spatial structure of  $X_j$  on  $\hat{\phi}_j$ . Commonly used are generalized ridge-type quadratic penalties (also called the “kernelizing approach”) and lasso-type  $\ell_1$ -penalties. The original APC proposal in [Donnell et al. \(1994\)](#) uses subspace regularization for estimation without providing asymptotic theory for it. In the present article we propose APCs based on shrinkage/kernelizing regularization and provide some asymptotic consistency theory.

It should be pointed out that introducing a shrinkage/kernelizing approach into a multivariate method is not a mechanical exercise. It is not a priori clear where and how the penalties should be inserted into a criterion of multivariate analysis, which in the case of PCA is variance subject to a constraint. The situation differs from regression where there is no conceptual difficulty in adding a regularization penalty to a goodness-of-fit measure. In a PCA-like method such as APC analysis, however, it is not clear whether penalties should be added to, or subtracted from, the variance, or somehow added to the constraint, or both. An interesting and related situation occurred in functional multivariate analysis where the same author (B. Silverman) co-authored two different approaches to the same PCA regularization problem ([Rice and Silverman, 1991](#); [Silverman, 1996](#)),

differing in where and how the penalty is inserted. Our approach, if transposed to functional multivariate analysis, agrees with neither of them. One reason for our third way is that neither of the approaches in [Rice and Silverman \(1991\)](#) or [Silverman \(1996\)](#) generalize to the low end of the PCA spectrum. In contrast, the regularized criterion proposed in this article can be applied to the high and the low end of the spectrum, and hence to the discovery of low dimension as well as low co-dimension. Our more specific interest is in the latter.

An immediate benefit of injecting penalty regularization into multivariate analysis stems from recent methodological innovations in kernelizing. These include the possibility of using infinite-dimensional function spaces, the interpretation of regularization kernels as positive definite similarity measures, and the kernel algebra with the freedom of modeling its engenders. Two decades ago, when [Donnell et al. \(1994\)](#) was written, it would have been harder to make the case for penalty regularization.

In what follows we first describe the mathematical structure of APCs which sets up the optimization problem that will be studied subsequently (Section 2). Section 3 discusses methodology for selecting penalty parameters in kernelized finite-sample APCs. In Section 4 we demonstrate the application of kernelized APC analysis in simulated and real data sets. Section 5 poses the APC problem in the framework of reproducing kernel Hilbert spaces. Section 6 establishes the existence of population APCs and the consistency of kernelized finite-sample APCs. Section 7 presents the power method for computing APCs, together with its supporting theoretical framework. We conclude with a discussion in Section 8. Proofs of results stated in Section 6 are in Appendix A, whereas proofs related to the power method of Section 7 are in Appendix B. Appendix C contains implementation details for the power method, while Appendix D contains an alternative linear algebra method for computing APCs.

## 2 Detailed Statement of the APC Problem

### 2.1 Transformations and Their Interpretations

The raw material for LPCs are real-valued random variables  $X_1, \dots, X_p$  with a joint distribution and finite second moments. LPCs are then defined as linear combinations  $\sum a_j X_j$  with extremal or stationary variance subject to a constraint  $\sum a_j^2 = 1$ .

For APCs one replaces linear combinations with additive combinations of the form  $\sum \phi_j(X_j)$  where  $\phi_j(X_j)$  are real-valued functions defined on arbitrary types of random observations  $X_j$ . That is,  $X_1, \dots, X_p$  can be random observations with values in arbitrary measurable spaces  $\mathcal{X}_1, \dots, \mathcal{X}_p$ , each of which can be continuous or discrete, temporal or spatial, high- or low-dimensional. The only assumption at this point is that these random observations have a joint distribution  $P_{1:p}(dx_1, \dots, dx_p)$  on  $\mathcal{X}_1 \times \dots \times \mathcal{X}_p$ . Random variables are obtained by forming real-valued functions  $\phi_j(X_j)$  of the arbitrarily-valued  $X_j$ . The functions  $\phi_j$  are often interpreted as “quantifications” or “scorings” or “scalings” of the underlying spaces  $\mathcal{X}_j$ . If  $X_j$  is already real-valued, then  $\phi_j(X_j)$  is interpreted as a variable transformation.

We will only consider functions  $\phi_j(X_j)$  that have finite variance and belong to some closed subspace of square-integrable functions with regard to their marginal distributions  $P_j(dx_j)$ :

$$\phi_j \in H_j \subset L^2(\mathcal{X}_j, dP_j) := \{\phi_j : \text{Var}(\phi_j(X_j)) < \infty\}.$$

In what follows we will write  $\phi_j$  or  $\phi_j(X_j)$  interchangeably. The role of the coefficient vector  $\mathbf{a} = (a_1, \dots, a_p)^T$  in LPCs is taken on by a vector of transformations:

$$\Phi := (\phi_1, \dots, \phi_p) \in \mathbf{H} := H_1 \times H_2 \times \dots \times H_p.$$

Similarly, the role of the linear combination  $\sum a_j X_j$  in LPCs is taken on by an additive function  $\sum \phi_j(X_j)$ . APCs contain LPCs as a special case when all  $X_j$  are real-valued and  $H_j = \{\phi_j : \phi_j(X_j) = a_j X_j, a_j \in \mathbb{R}\}$ .

## 2.2 Population Inner Products and Irrelevant Constants

The inner product will initially be population covariance. For this reason all functions are defined only modulo sets of measure zero and also modulo constants. Constants are a particular nuisance in additive functions  $\sum \phi_j$  because they are non-identifiable across the transformations: for example,  $\tilde{\phi}_k = \phi_k + c$ ,  $\tilde{\phi}_l = \phi_l - c$  for some  $k \neq l$  and  $\tilde{\phi}_j = \phi_j$  else result in the same additive function,  $\sum \tilde{\phi}_j = \sum \phi_j$ .

To deal with unidentifiable constants in additive functions, we think of  $L^2(\mathcal{X}_j, dP_j)$  as consisting of equivalence classes of functions where two functions are equivalent if they differ by a function that is constant almost everywhere (rather than requiring the two functions to be equal almost everywhere). We can then endow  $H_j$  with the covariance as inner product and the variance as the squared norm:

$$\langle \phi_j, \psi_j \rangle_{P_j} := \text{Cov}(\phi_j, \psi_j) \quad \text{and} \quad \|\phi_j\|_{P_j}^2 := \text{Var}(\phi_j).$$

The natural inner product and squared norm on the product space  $\mathbf{H}$  are therefore

$$\langle \Phi, \Psi \rangle_{P_{1:p}} := \sum_{j=1}^p \langle \phi_j, \psi_j \rangle_{P_j} \quad \text{and} \quad \|\Phi\|_{P_{1:p}}^2 := \sum_{j=1}^p \|\phi_j\|_{P_j}^2.$$

To avoid unidentifiable constants, [Donnell et al. \(1994\)](#) take  $H_j$  to be a closed subspace of centered transformations,  $L_c^2(\mathcal{X}_j, dP_j) := \{\phi_j : E\phi_j = 0, \text{Var}(\phi_j) < \infty\}$ . This solution to the non-identifiability problem of constants is essentially equivalent to ours, but ours has the benefit that it does not raise unnecessary questions when estimates  $\hat{\phi}_j$  of the transformations  $\phi_j$  cannot be centered at the population (which is not known) and hence strictly speaking cannot be in  $H_j$  as defined in [Donnell et al. \(1994\)](#). Our framework says that differences by constants are irrelevant and should be ignored.

## 2.3 Criterion and Constraint — A Null Comparison Principle

In the introduction we stated that the optimization criterion for APCs is variance,  $\text{Var}(\sum \phi_j)$ , but we did not specify the normalization constraint other than writing it as  $\sum \|\phi_j\|^2 = 1$ . From the previous subsections it is clear that we will choose the constraint norms to be  $\|\phi_j\|_{P_j}^2 = \text{Var}(\phi_j)$ . This was the choice made by [Donnell et al. \(1994\)](#), their justification being that it generalizes LPCs: for  $H_j = \{a_j X_j : a_j \in \mathbb{R}\}$  we have  $\text{Var}(\phi_j) = a_j^2$  for real-valued standardized  $X_j$ ,  $\text{Var}(X_j) = 1$ , hence the constraint becomes  $\sum a_j^2 = 1$ .

To kernelize APCs, we will need a deeper justification for the constraint. Even for LPCs, however, we may ask: what is it that makes  $\sum a_j^2$  “natural” as a quadratic constraint form? The answer we propose is in the following:

***Null comparison principle for multivariate analysis:*** *The quadratic form to be used for the constraint is the optimization criterion evaluated under the null assumption of vanishing correlations.*

This principle ties the constraint form in a unique way to the criterion: There is no longer a choice of the constraint because it derives directly from the criterion. We arrive at a powerful

and principled way of devising generalizations of multivariate methods, as will be exemplified when we kernelize APCs. For the familiar cases the principle works out as follows: For LPCs the null assumption is

$$\text{Cov}(X_j, X_k) = 0 \quad \forall j \neq k.$$

The evaluation of the criterion, assuming also standardized real variables  $X_j$ , results in the familiar form

$$\text{Var}(\sum a_j X_j) = \sum \text{Var}(a_j X_j) = \sum a_j^2.$$

For APCs the null assumption is

$$\text{Cov}(\phi_j(X_j), \phi_k(X_k)) = 0 \quad \forall \phi_j \in H_j, \phi_k \in H_k, j \neq k,$$

that is, pairwise independence of the  $X_j$ . The evaluation of the criterion results in

$$\text{Var}(\sum \phi_j(X_j)) = \sum \text{Var}(\phi_j(X_j)),$$

agreeing with our choice for the constraint form. In retrospect this justifies what we defined above to be the “natural” squared norm on  $\mathbf{H} = H_1 \times \cdots \times H_p$ . Associated with it is the “natural” inner product also defined above:

$$\langle \Phi, \Psi \rangle_{P_{1:p}} = \sum \text{Cov}(\phi_j(X_j), \psi_j(X_j)).$$

Its utility is in defining hierarchies of APCs whereby the constrained optimization problem is solved repeatedly under the additional constraint of orthogonality to all previously obtained solutions.

## 2.4 Kernelized APCs

The APC estimation procedure of [Donnell et al. \(1994\)](#) can be characterized as using the above APC framework where one replaces the population distribution  $P_{1:p}$  with the empirical distribution  $\hat{P}_{1:p} = \frac{1}{n} \sum_i \delta_{\mathbf{x}_i}$  of the data  $\{\mathbf{x}_i : 1 \leq i \leq n\}$ , and  $H_j$  by finite-dimensional Hilbert spaces  $\hat{H}_j$  whose dimension is low compared to  $n$  (they may be spanned by dummy variables for discrete  $X_j$  or by low-degree monomials or spline basis functions with few knots for quantitative  $X_j$ ). The finite dimensionality of the spaces  $\hat{H}_j$  achieves the regularization necessary for estimation. The empirically solvable optimization problem is therefore

$$\min_{\phi_j \in \hat{H}_j} \widehat{\text{Var}}\left(\sum_{j=1}^p \phi_j\right) \quad \text{subject to} \quad \sum_{j=1}^p \widehat{\text{Var}}(\phi_j) = 1, \quad (1)$$

where  $\widehat{\text{Var}}$  is the empirical variance obtained from data. This reduces to a generalized finite-dimensional eigenvalue/eigenvector problem ([Donnell et al., 1994](#)).

By contrast, we will consider here APC estimation based on kernelizing, where regularization is achieved through additive quadratic penalties  $J_j(\phi_j)$  that induce Reproducing Kernel Hilbert Spaces (RKHS)  $\mathcal{H}_j$  which become the natural choice for  $H_j$ . While estimation is again based on the empirical distribution  $\hat{P}_{1:p}$ , a regularized population version based on the actual distribution  $P_{1:p}$  exists also and is useful for bias-variance calculations. For simplicity of notation we continue the discussion for the population case. The kernelized optimization criterion we choose is the penalized variance:

$$\text{Var}\left(\sum_{j=1}^p \phi_j\right) + \sum_{j=1}^p J_j(\phi_j). \quad (2)$$

This is a natural choice for minimization because it forces the transformations  $\phi_j$  not only to generate small variance but also regularity in the sense of the penalties. For concreteness the reader may use as a leading example a cubic spline penalty  $J_j(\phi_j) = \alpha_j \int \phi_j''(x_j) dx_j$  for a quantitative variable  $X_j$  (where we absorbed the tuning constant  $\alpha_j$  in  $J_j$ ), but the reader versed in kernelizing will recognize the generality of modeling offered by positive definite quadratic forms that generate RKHSs.

The question is next what the natural constraint should be. Informed by the null comparison principle of Section 2.3, we will not naively carry  $\sum \text{Var}(\phi_j) = 1$  over to the kernelized problem. Instead we evaluate the criterion (2) under the assumption of absent correlations between the transformations  $\phi_j$  in the spaces  $\mathcal{H}_j$ :

$$\sum_{j=1}^p \text{Var}(\phi_j) + \sum_{j=1}^p J_j(\phi_j) = 1. \quad (3)$$

As it turns out, this formulation produces meaningful results both for minimization *and* maximization, hence both for estimating implicit additive equations for discovery of structure of *low co-dimension*, and for estimating additive dimension reduction for discovery of structure of *low dimension*. In the present article we pursue the former goal. — An equivalent unconstrained problem is in terms of the associated Rayleigh quotient:

$$\min/\max/\text{stationary}_{\phi_1, \dots, \phi_p} \frac{\text{Var}(\sum \phi_j) + \sum J_j(\phi_j)}{\sum \text{Var}(\phi_j) + \sum J_j(\phi_j)} \quad (4)$$

On data we will replace the population quantities in equations (2) and (3) with their sample counterparts. As is usual, the penalties will be expressed in terms of quadratic forms of certain kernel matrices.

## 2.5 Alternative Approaches to Kernelized APCs

A brief historic digression is useful to indicate the conceptual problem solved by the null comparison principle: As mentioned in the introduction, in the related but different field of functional multivariate analysis, Silverman co-authored two different approaches to the same PCA regularization problem where largest principal components are sought for dimension reduction. These can be transposed to the APC problems as follows:

$$\max_{\phi_1, \dots, \phi_p} \text{Var}(\sum \phi_j) - \sum J_j(\phi_j) \quad \text{subject to} \quad \sum \text{Var}(\phi_j) = 1, \quad (5)$$

$$\max_{\phi_1, \dots, \phi_p} \text{Var}(\sum \phi_j) \quad \text{subject to} \quad \sum \text{Var}(\phi_j) + \sum J_j(\phi_j) = 1, \quad (6)$$

where (5) is due to Rice and Silverman (1991) and (6) is due to Silverman (1996). The first approach (5) subtracts the penalty from the criterion, which does what it should do for regularized variance *maximization*. It is unsatisfactory for reasons of mathematical aesthetics: a difference of two quadratic forms can result in negative values, which may not be a practical problem but “does not seem right’.” The second approach (6) solves this issue by adding a penalty to the constraint rather than subtracting it from the criterion, which again does what it should do for variance maximization. Both approaches can be criticized for resulting in non-sense when the goal is regularized variance *minimization*. Here the first approach (5) is more satisfying because it is immediately clear how to modify it to work for regularized variance minimization:

$$\min_{\phi_1, \dots, \phi_p} \text{Var}(\sum \phi_j) + \sum J_j(\phi_j) \quad \text{subject to} \quad \sum \text{Var}(\phi_j) = 1,$$

whereas for the approach (6) it is not clear how it could be modified to work in this case. Subtracting the penalty from the constraint variance,  $\sum \text{Var}(\phi_j) - \sum J_j(\phi_j) = 1$ , is clearly not going to work.

Escewing these problems, we propose

$$\min_{\phi_1, \dots, \phi_p} \text{Var}(\sum \phi_j) + \sum J_j(\phi_j) \quad \text{subject to} \quad \sum \text{Var}(\phi_j) + \sum J_j(\phi_j) = 1. \quad (7)$$

The merits of this proposal are that (1) it has no aesthetic issues, (2) it works for both ends of the variance spectrum, and (3) it derives from a more fundamental principle rather than mathematical experimentation.

## 2.6 The Kernelizing View of APCs

The major benefit of formulating APCs in the kernelizing framework is the flexibility of embedding the information contained in data objects in  $p$  different  $n \times n$  kernel matrices as opposed to an  $n \times p$  feature matrix. Kernel matrices have an interpretation as similarity measures between pairs of data objects. It is therefore possible to directly design similarity matrices (instead of features) for non-Euclidean data for use as kernels. Thus topological information between data objects captured by kernels can be used to directly estimate APC transforms of non-quantitative data. Just as one extracts multiple features from data objects, one similarly extracts multiple similarity matrices to capture different topological information in data objects. APC then helps us find associations between these kernels in terms of “implicit” redundancies. Following the discussion at the end of Section 2.4, on data the APC variance is evaluated on the sum of transforms, and the penalties are obtained from the constructed kernel matrices.

## 2.7 Relation of APCs to Other Kernelized Multivariate Methods

The focus on the lower end of the spectrum seems to have found little attention in the literature, but the criterion we use can be related to existing proposals even if their focus is on the upper end of the spectrum.

A special situation with precedent in the literature occurs for  $p = 2$ , in which case the kernelized APC problem (7) reduces to the kernelized canonical correlation analysis (CCA) problem discussed by Fukumizu et al. (2007). To see the equivalence, one may start with the simplified Rayleigh problem (4),

$$\min/\max/\text{stationary}_{\phi_1, \phi_2} \frac{\text{Var}(\phi_1 + \phi_2) + J_1(\phi_1) + J_2(\phi_2)}{\text{Var}(\phi_1) + \text{Var}(\phi_2) + J_1(\phi_1) + J_2(\phi_2)}. \quad (8)$$

It can be shown that stationary solutions satisfy

$$\text{Var}(\phi_1) + J_1(\phi_1) = \text{Var}(\phi_2) + J_2(\phi_2), \quad (9)$$

and it follows that the problem (8) is equivalent to

$$\min/\max/\text{stationary}_{\phi_1, \phi_2} \frac{\text{Cov}(\phi_1, \phi_2)}{(\text{Var}(\phi_1) + J_1(\phi_1))^{1/2} (\text{Var}(\phi_2) + J_2(\phi_2))^{1/2}},$$

where the normalization (9) can be enforced without loss of generality. This is recognized as a penalized form of CCA. It has been rediscovered several times over, in the machine learning literature by Bach and Jordan (2003), and earlier in the context of functional multivariate analysis by Leurgans et al. (1993).



Interesting is the work of [Bach and Jordan \(2003\)](#) which generalizes CCA to the case  $p > 2$  but shows no interest in the results of such an analysis other than this becoming the building block in a method for independent components analysis (ICA), where the input variables  $X_j$  are projections of multivariate data onto frames of orthogonal unit vectors. [Bach and Jordan \(2003\)](#) correctly build up a finite-sample version of what amounts to APCs for  $p > 2$  without a guiding principle other than the appearance of it being a “natural generalization”. A population version and associated consistency theory is missing as their focus is on ICA and associated computational problems.

Finally it would be natural to discuss a relationship between kernel APCs and kernel principal components (KPCA, [Schölkopf et al. \(1998\)](#), [Schölkopf and Smola \(2002\)](#)). However, we do not see a natural connection at this point.

### 3 Methodologies for Choosing Penalty Parameters

Any kernel calls implicitly for a multiplicative penalty parameter that controls the amount of regularization to balance bias and variance against each other. Methods that use multiple kernels will have as many penalty parameters as kernels. Choosing these parameters in a given problem requires some principles for systematically selecting the values for these parameters. Such principles have been discussed at least as long as there have existed additive models ([Hastie and Tibshirani, 1990](#)), and APCs pose new problems only in so far as they use Rayleigh quotients as their optimization criteria rather than residual sums of squares or other regression loss functions as their minimization criteria. An initial division of principles for penalty parameter selection is into a priori choice and data-driven choice.

#### 3.1 A Priori Choice of Penalty Parameters

In order to make an informed a priori choice of a penalty parameter it must be translated into an interpretable form. The most common such form is in terms of a notion of “degrees of freedom” which can be heuristically rendered as “equivalent number of observations invested in estimating a transformation.” To define degrees of freedom for kernelizing one makes use of the fact that for a fixed penalty parameter a fit  $\hat{\phi}^{(n)}(x)$  produced by a kernel on regressor-response data  $(x_i, y_i)$  of size  $n$  is a linear operation  $\mathbf{y} = (y_i)_{i=1\dots n} \mapsto \hat{\phi}^{(n)}$ ,  $\mathbb{R}^n \rightarrow H$ , hence the evaluation map  $\mathbf{y} \mapsto \hat{\mathbf{y}} = (\hat{\phi}^{(n)}(x_i))_{i=1\dots n}$ ,  $\mathbb{R}^n \rightarrow \mathbb{R}^n$  can be represented by a matrix operation  $\mathbf{S}\mathbf{y} = \hat{\mathbf{y}}$ , where the  $n \times n$  “smoother matrix”  $\mathbf{S}$  is symmetric and non-negative definite, and all its eigenvalues are  $\leq 1$ . The matrix  $\mathbf{S}$  depends on the penalty parameter  $\alpha$ ,  $\mathbf{S} = \mathbf{S}_\alpha$ , and serves as the basis for defining notions of degrees of freedom. Several definitions exist, three of which are as follows ([Buja et al., 1989](#)):

- $df = \text{tr}(\mathbf{S}^2)$ : This derives from the total variance in  $\hat{\mathbf{y}}$ , which under homoskedasticity is  $\sum_i \text{Var}(\hat{y}_i) = \text{tr}(\mathbf{S}\mathbf{S}')\sigma^2$ . Variance of fitted values is a measure of how much response variation has been invested in the fits.
- $df = \text{tr}(2\mathbf{S} - \mathbf{S}^2)$ : This derives from the total residual variance in  $\mathbf{r} = \mathbf{y} - \hat{\mathbf{y}}$  under a homoskedasticity assumption:  $\sum_i \text{Var}(r_i) = \text{tr}(\mathbf{I} - \mathbf{S} - \mathbf{S}' + \mathbf{S}\mathbf{S}')\sigma^2$ . Variance of residuals, when subtracted from  $n\sigma^2$ , is a measure of how much of the error variance has been lost to the fitted values.
- $df = \text{tr}(\mathbf{S})$ : This derives from a Bayesian interpretation of kernelizing under a natural Bayes prior that results in  $\mathbf{S}\sigma^2$  as the posterior covariance matrix of  $\hat{\mathbf{y}}$ . A frequentist derivation is obtained by generalizing Mallows’  $C_p$  statistic which corrects the residual sum of squares with



a term  $2(df)\hat{\sigma}^2$  to make it unbiased for the predictive MSE; the appropriate generalization for smoothers is  $df = \text{tr}(\mathbf{S})$ .

Among these, the third is the most popular version. If  $\mathbf{S}$  is a projection, all three definitions result in the same value, which is the projection dimension, but for kernels whose  $\mathbf{S}$  contains eigenvalues strictly between 0 and 1 the three definitions are measures of different concepts. For general kernels the calculation of degrees of freedom for a ladder of penalty parameter values  $\alpha$  may result in considerable computational expense, which is compounded by the fact that in practice for a prescribed degree of freedom several values of  $\alpha$  need to be tried in a bisection search. Yet the translation of  $\alpha$  to a degree of freedom may be the most natural device for deciding a priori on an approximate value of the penalty parameter. Selecting degrees of freedom separately for each transformation  $\phi_j$  is of course a heuristic for APCs, as it is for additive regression models, because what matters effectively is the total degrees of freedom in the additive function  $\sum_{j=1}^p \hat{\phi}_j^{(n)}$ . Summing up the individual degrees of freedom of  $\hat{\phi}_j^{(n)}$  is only an approximation to the degrees of freedom of  $\sum_{j=1}^p \hat{\phi}_j^{(n)}$  (Buja et al., 1989).

In practice one often decides on identical degrees of freedom  $df$  for all transforms  $\hat{\phi}_j^{(n)}$  and chooses the sum  $p \cdot df$  to be a fraction of  $n$ , such as  $p \cdot df = n/10$ .

### 3.2 Data-driven Choice of Penalty Parameters

The most popular data-driven method is based on cross-validation. A first question is what the criterion should be that is being cross-validated. We use as the relevant criterion the empirical, unpenalized sample eigenvalue:

$$\hat{\lambda}_1 := \frac{\widehat{\text{Var}}(\sum \hat{\phi}_j)}{\sum \widehat{\text{Var}}(\hat{\phi}_j)}.$$

It is an estimate of  $\lambda_1 := \min_{\phi_1, \dots, \phi_p} \text{Var}(\sum \phi_j) / \sum \text{Var}(\phi_j)$  which, when small ( $\ll 1$ ), suggests the existence of concavity in the data. Of course, the criterion that is actually being minimized is the penalized sample eigenvalue:

$$\frac{\widehat{\text{Var}}(\sum \hat{\phi}_j) + \sum J_j(\hat{\phi}_j)}{\sum \widehat{\text{Var}}(\hat{\phi}_j) + \sum J_j(\hat{\phi}_j)}.$$

This we treat as a surrogate quantity that is not of substantive interest. (The distinction between quantity of interest and surrogate quantity is familiar from supervised classification where interest focuses on misclassification rates but minimization is carried out on surrogate loss functions such as logistic or exponential loss; accordingly it is misclassification rates that are used in cross-validation.)

To choose the penalty parameters in the simplest possible way, one often makes them identical for all variables and then searches their common value  $\alpha$  on a grid, minimizing the  $k$ -fold cross-validation criterion

$$\text{CV}(\alpha) = \frac{1}{k} \sum_{i=1}^k \frac{\widehat{\text{Var}}(\sum_{j=1}^p \hat{\phi}_{\{i\}j})}{\sum_{j=1}^p \widehat{\text{Var}}(\hat{\phi}_{\{i\}j})}.$$

The variances  $\widehat{\text{Var}}$  are evaluated on the holdout sets while the transforms  $\hat{\phi}_{\{i\}j}$  are estimated from the training sets.

Here, however, attention must be paid to the question of what “equal value of the penalty parameters” means. The issue is that the meaning of a penalty parameter  $\alpha$  is very much scale dependent. For example, a standard Gaussian kernel  $k(x, x') = \exp\{-\frac{1}{2}(x - x')^2\}$  is very different when a variable measured in miles is converted to a variable measured in feet. One approach to

equalizing the effect of scale on the penalties and kernels is to standardize all variables involved. Another approach is to calibrate all penalty parameters to produce the same degrees of freedom.

## 4 Simulation and Application to Real Data

In this section we demonstrate the use of APC in identifying additive degeneracy in data. We first apply APC analysis to a university webpages data and an air pollution data. We then evaluate the finite-sample performance of APC on a simulated data for which the optimal transformations are known.

### 4.1 Real Data

#### 4.1.1 University Webpages

In this section, we demonstrate the kernelizing use of kernel APC in estimating additive implicit equation. Instead of extracting features and estimating APC transforms of the features, we start with similarity measures between data points and use them as elements in the kernel matrices directly. In this case, one can view APC transformation as an embedding of the original data points in the Euclidean space into an RKHS, and the estimated additive constraints represent an implicit equation in the embedded space. Such flexibility is only possible with kernel APC (which only requires kernel matrices as input) but not with the original subspace restriction APC as considered in [Donnell et al. \(1994\)](#) (which requires a specification of basis functions as input).

group 1		group 2	group 3		group 4	
activ	student	address	acm	languag	advanc	receiv
area	teach	contact	algorithm	method	assist	scienc
book	work	cours	analysi	model	associ	softwar
build	year	depart	applic	network	center	state
california		email	architectur	parallel	colleg	technolog
chair		fall	base	problem	degre	univers
class		fax	comput	process	director	
current		hall	confer	program	educ	
faculti		home	data	public	electr	
graduat		inform	design	research	engin	
group		link	develop	select	institut	
includ		list	distribut	structur	intellig	
interest		mail	gener	studi	laboratori	
introduc		offic	high	system	mathemat	
paper		page	ieee	techniqu	member	
project		phone	implement	theori	number	
recent		updat	investig	time	profession	
special		web	journal	tool	professor	

Table 1: Keywords in group 1 to group 4.

We consider the university webpages data set from the “World Wide Knowledge Base” project at Carnegie Mellon University. This data set was preprocessed by [Cardoso-Cachopo \(2009\)](#) and previously studied in [Guo et al. \(2011\)](#) and [Tan et al. \(2015\)](#). It includes webpages from computer science departments at Cornell, University of Texas, University of Washington, and University of

Wisconsin. In this analysis, we consider only the faculty webpages — resulting in  $n = 374$  faculty webpages and  $d = 3901$  keywords that appear on these webpages.

We now discuss how we constructed for this data set four similarity matrices to be used as kernels. First we reduced the number of keywords from 3901 to 100 by thresholding the log-entropy. Let  $f_{ij}$  be the number of times the  $j^{th}$  keyword appears in the  $i^{th}$  webpage. The log-entropy of the  $j^{th}$  keyword is defined as  $1 + \sum_{i=1}^n g_{ij} \log(g_{ij}) / \log(n)$ , where  $g_{ij} = f_{ij} / \sum_{i=1}^n f_{ij}$ . We then selected the 100 keywords with the largest log-entropy values and constructed an  $n \times 100$  matrix  $H$  whose  $(i, j)$  element is  $\log(1 + f_{ij})$ . We further standardized each column to have zero mean and unit variance. In order to obtain four different kernels, we applied the  $k$ -means algorithm to cluster the keywords in  $H$  into  $k = p = 4$  groups. Each group of keywords is represented as an  $n \times m_i$  submatrix  $H_i$ , and we obtained the final  $n \times n$  kernel matrix  $K_i = H_i H_i^T / \text{tr}(H_i H_i^T)$ , where the normalization is to account for different group sizes. Table 1 shows the keywords in each group. Roughly, group 1 contains keywords related to teaching and current projects, group 2 contains keywords related to contact information, group 3 contains keywords related to research area, and group 4 contains keywords related to biography of a faculty.

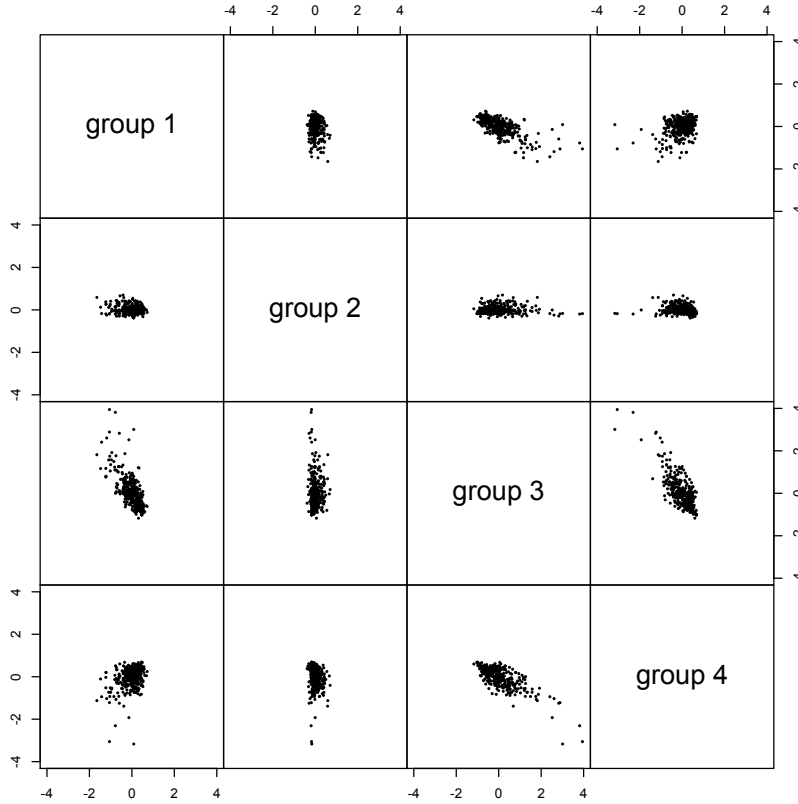


Figure 1: Pairwise scatterplot of the smallest kernelized sample APC for the university webpages data. The sample eigenvalue for the estimated APC is 0.0910.

Upon an APC analysis using the kernel matrices  $K_1, \dots, K_4$  constructed above, we obtain the transformations  $\hat{\phi}_1, \dots, \hat{\phi}_4$ . Figure 1 shows the pairwise scatterplot of the transformed data points. We see that  $\hat{\phi}_3$  and  $\hat{\phi}_4$  have strong negative correlation,  $\hat{\phi}_1$  and  $\hat{\phi}_3$  have moderate negative correlation, and  $\hat{\phi}_1$  and  $\hat{\phi}_4$  have weak positive correlation. For ease of interpretation, the transformed

data points are centered to zero mean and normalized to  $\sum_{j=1}^4 \widehat{\text{Var}} \hat{\phi}_j = 1$ . The normalization permits us to interpret  $\widehat{\text{Var}} \hat{\phi}_j$  as relative importance of the  $j^{\text{th}}$  group in the estimated APCs. The variance of each group in the smallest APC are: 0.1662 (group 1), 0.0305 (group 2), 0.5562 (group 3), 0.2471 (group 4). Ignoring group 2 which has the smallest weight, we see that, roughly, this means that

$$\hat{\phi}_1 + \hat{\phi}_3 + \hat{\phi}_4 \approx 0, \quad \text{or, equivalently,} \quad \hat{\phi}_4 \approx -\hat{\phi}_1 - \hat{\phi}_3.$$

If we plot  $\hat{\phi}_4$  against  $\hat{\phi}_1 + \hat{\phi}_3$ , we get the scatterplot in Figure 2.

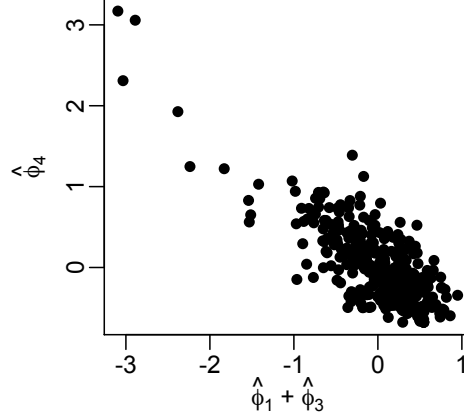


Figure 2: Plot of  $\hat{\phi}_4$  against  $\hat{\phi}_1 + \hat{\phi}_3$  in the smallest kernelized sample APC for the university webpages data.

Recalling that the kernels were constructed to reflect similarity in terms of keywords related to (1) teaching and current projects, (2) contact information, (3) research area, and (4) biography, we obtain two results: contact information is related to neither of teaching and projects nor research, whereas biography is well predicted by teaching, projects and research. This is of course highly plausible for faculty webpages and academic biographies.

#### 4.1.2 Air Pollution

In this section, we apply APC analysis to a data set consisting of quantitative variables, where the purpose is to find nonlinear transformations that reflect redundancies among the variables. To this end we analyze the  $NO_2$  data that is publicly available on the StatLib data sets archive <http://lib.stat.cmu.edu/datasets/NO2.dat>. It contains a subsample of 500 observations from a data set collected by the Norwegian Public Roads Administration for studying the dependence of air pollution at a road on traffic volume and meteorological condition. The response variable consists of hourly values of the log-concentration of  $NO_2$  particles, measured at Alnabru in Oslo, Norway, between October 2001 and August 2003. Because the posted data is only a subset of the original data, the middle chunk of observations is missing. To avoid nonsensical transformations of the variables, only the second half of the data (roughly November 2002 to May 2003) is used in the APC analysis. Given below are descriptions for individual variables in the data:

NO2: hourly values of the logarithm of the concentration of  $NO_2$  particles;  
 Cars: logarithm of the number of cars per hour;  
 TempAbove: temperature 2 meter above ground (degree C);  
 Wind: wind speed (meters/second);  
 TempDiff: temperature difference between 25 and 2 meters above ground (degree C);  
 WindDir: wind direction (degrees between 0 and 360);  
 HourOfDay: hour of day;  
 DayNumber: day number from October 1, 2001.

Figure 3 shows the corresponding transformations for individual variables in the smallest APC. The variables **Cars** and **HourOfDay** are the primary variables involved (with respective variance 0.51 and 0.304). Holding other variables fixed, the estimated constraint says that  $\hat{\phi}_2(\text{Cars}) + \hat{\phi}_7(\text{HourOfDay}) \approx 0$ . Since  $\hat{\phi}_2$  is monotone decreasing and the transformation of **HourOfDay** peaks around 4pm, we infer that the largest number of cars on the roads is found in the late afternoon, which is consistent with the daily experience of commuters.

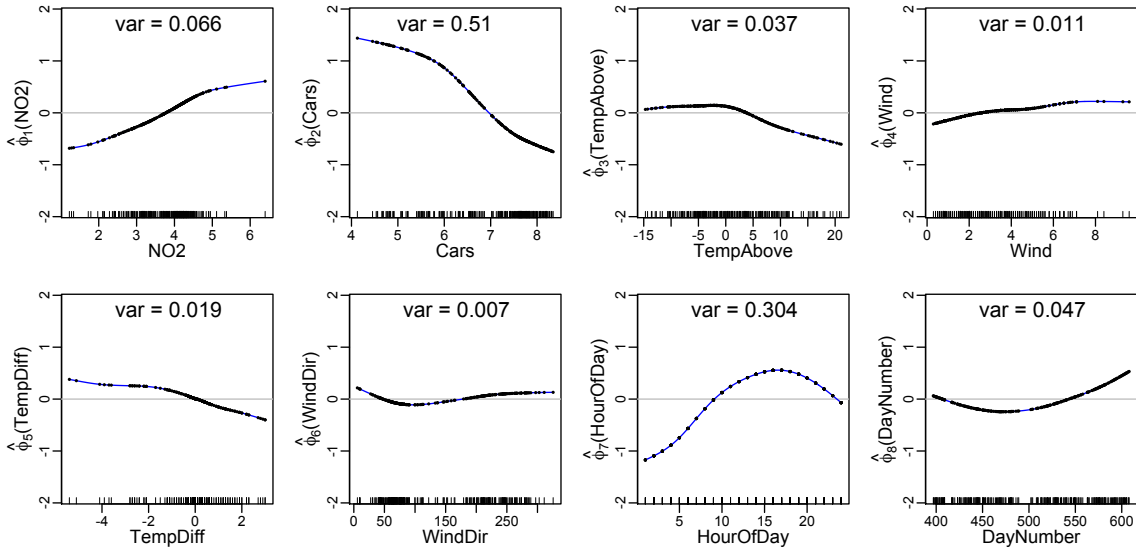


Figure 3: The smallest kernelized sample APC for the  $NO_2$  data obtained from power algorithm using Sobolev kernel for individual variables. The sample eigenvalue for the estimated APC is 0.0621. The black bars at the bottom of each plot indicate the location of data points for that variable.

In the second smallest APC in Figure 4, the variables **TempAbove** and **DayNumber** play the dominant roles, and we have  $\hat{\phi}_3(\text{TempAbove}) + \hat{\phi}_8(\text{DayNumber}) \approx 0$ . Since  $\hat{\phi}_3$  is monotone decreasing it follows that **TempAbove** decreases and then increases with respect to **DayNumber**. This relationship makes sense since our data spans over November 2002 to May 2003, hence carries the transition from fall to summer.

The response variable of interest in the original study, **NO2**, does not appear until the third smallest APC, which is given in Figure 5. We have  $\hat{\phi}_1(\text{NO2}) + \hat{\phi}_5(\text{TempDiff}) + \hat{\phi}_7(\text{HourOfDay}) \approx 0$ . From the shape of  $\hat{\phi}_7$  we see that the highest **NO2** occurs during lunch time, which makes sense as this is the time of greatest sun exposure. Note that surprisingly there is no interpretable association with **Cars** as its transformation has little variance and is not monotone (more cars should create more **NO2**). However, the strong association between **Cars** and **HourOfDay** in the smallest APC

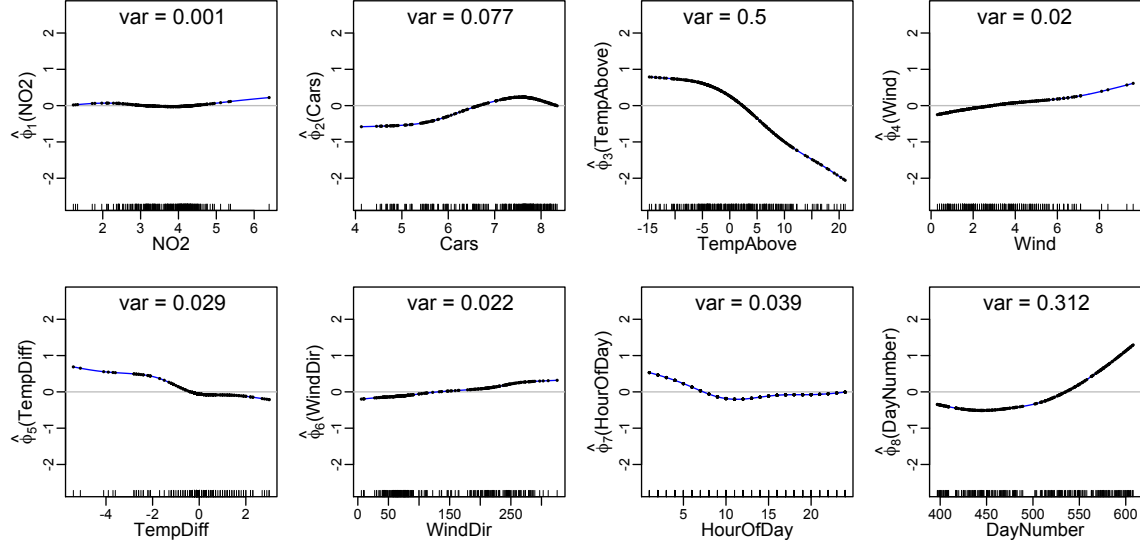


Figure 4: The second smallest kernelized sample APC for the  $NO_2$  data obtained from power algorithm using Sobolev kernel for individual variables. The sample eigenvalue for the estimated APC is 0.0827. The black bars at the bottom of each plot indicate the location of data points for that variable.

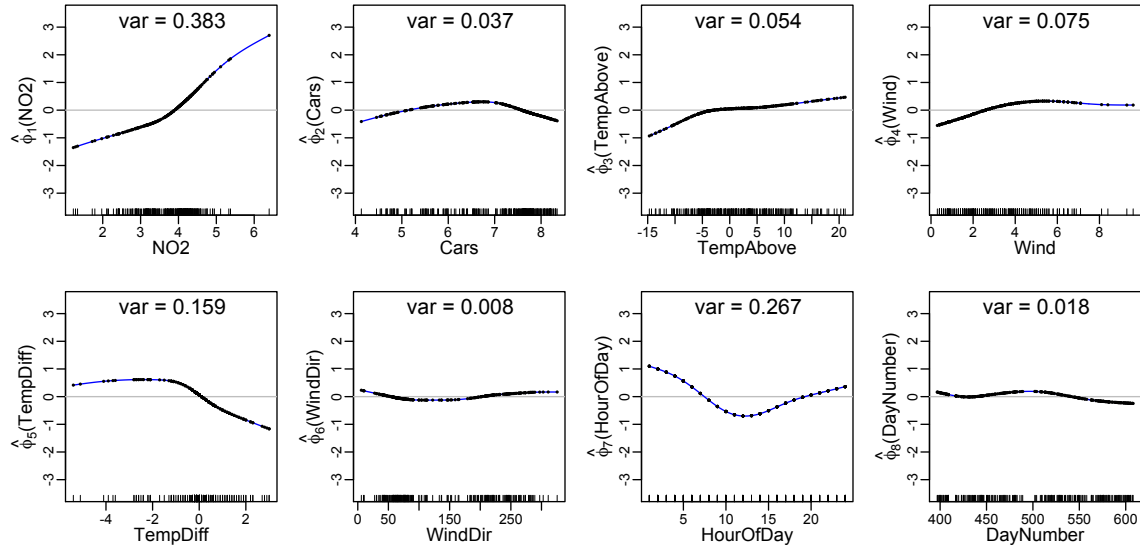


Figure 5: The third smallest kernelized sample APC for the  $NO_2$  data obtained from power algorithm using Sobolev kernel for individual variables. The sample eigenvalue for the estimated APC is 0.189. The black bars at the bottom of each plot indicate the location of data points for that variable.



creates an approximate non-identifiability of association of `Cars` and `HourOfDay` vis-à-vis other variables such as `N02`, which may partly explain the absence of association between `Cars` and `N02`.

APC analysis suggests some interesting relationship among the variables in the data. It also suggests that had an additive model been fitted to the data with `N02` as the response and all other variables as the predictors, the estimated transforms for individual variables will not be interpretable due to the presence of concurvity (as represented by the smallest and second smallest APC) in the data.

## 4.2 Simulated Data

We construct a simulated example consisting of four univariate random variables  $X_1, \dots, X_4$  with known APC transformations  $\phi_1(X_1), \dots, \phi_4(X_4)$ . This will be achieved by constructing them in such a way that the joint distribution of these transformations will be multivariate normal and highly collinear. The reason for this construction is that the extremal APCs of multivariate normal distributions are linear. (They also have APCs with non-extremal eigenvalues consisting of systems of Hermite polynomials; see [Donnell et al. \(1994\)](#).) This implies that if transformations  $\phi_j(X_j)$  exist that result in a jointly multivariate normal distribution, they will constitute an APC.

A simple procedure for simulating a situation with well-defined APCs is to first construct a multivariate normal distribution and transform its variables with the inverses of the desired transformations. APC estimation is then supposed to find approximations of these transformations from data simulated in this manner.

We start by constructing a multivariate normal distribution by using two independent variables  $W_1, W_2 \sim \mathcal{N}(0, 1)$  to generate the underlying collinearity and four independent variables  $Z_1, Z_2, Z_3, Z_4 \sim \mathcal{N}(0, 0.1^2)$  to generate noise:

$$Y_1 = W_1 + Z_1, \quad Y_2 = W_2 + Z_2, \quad Y_3 = W_1 + W_2 + Z_3, \quad Y_4 = Z_4.$$

Thus the joint distribution features a collinearity of co-dimension 1 in the first three variables, and the fourth variable is independent of the rest. The correlation matrix of these four variables has a smallest eigenvalue of 0.007441113..., which will be the smallest population APC eigenvalue. The associated eigenvector is  $(1/2, 1/2, 1/\sqrt{2}, 0)$ , which indicates that the fourth transform will be zero, whereas the first three transforms will have variances 1/4, 1/4 and 1/2, respectively. The “observed” variables are constructed as marginal transformations  $X_j = f_j(Y_j)$  using the following choices:

$$X_1 = \exp(Y_1), \quad X_2 = -Y_2^{1/3}, \quad X_3 = \exp(Y_3)/(1 + \exp(Y_3)), \quad X_4 = Y_4,$$

hence the APC transformations are

$$\phi_1^*(x) \sim \log(x), \quad \phi_2^*(x) \sim -x^3, \quad \phi_3^*(x) \sim \log(x/(1 - x)), \quad \phi_4^*(x) = 0.$$

As noted above the last transformation vanishes, and the other transformations are given only up to irrelevant additive constants as well as scales to achieve  $\text{Var}(\phi_1) = \text{Var}(\phi_2) = 1/4$  and  $\text{Var}(\phi_3) = 1/2$ .

Figure 6 shows the kernelized sample APC for this data set ( $n = 250$ ), with a common penalty parameter chosen by 5-fold cross-validation. As discussed at the end of Section 3.2, we standardized all variables to have unit variance before applying a standard Gaussian kernel  $k(x, x') = \exp\{-\frac{1}{2}(x - x')^2\}$  for each variable  $X_j$ . The solid red line denotes the true transform  $\phi_j^*$ , while the dashed blue line denotes estimated transform  $\hat{\phi}_j$ . We see that for each variable, the two lines are almost

indistinguishable, though estimation accuracy worsens near the boundaries and on regions with few data points (location of data points are indicated by the black bars at the bottom of each plot). The transformed data points are centered to zero mean and normalized to  $\sum_{j=1}^4 \widehat{\text{Var}} \hat{\phi}_j = 1$ , so that  $\widehat{\text{Var}} \hat{\phi}_j$  indicates the relative importance of  $\hat{\phi}_j$  in the estimated APCs. In fact, we see that  $\widehat{\text{Var}} \hat{\phi}_j$  is close to  $\text{Var} Y_j / (\sum_{i=1}^4 \text{Var} Y_i)$  in the data generating steps.

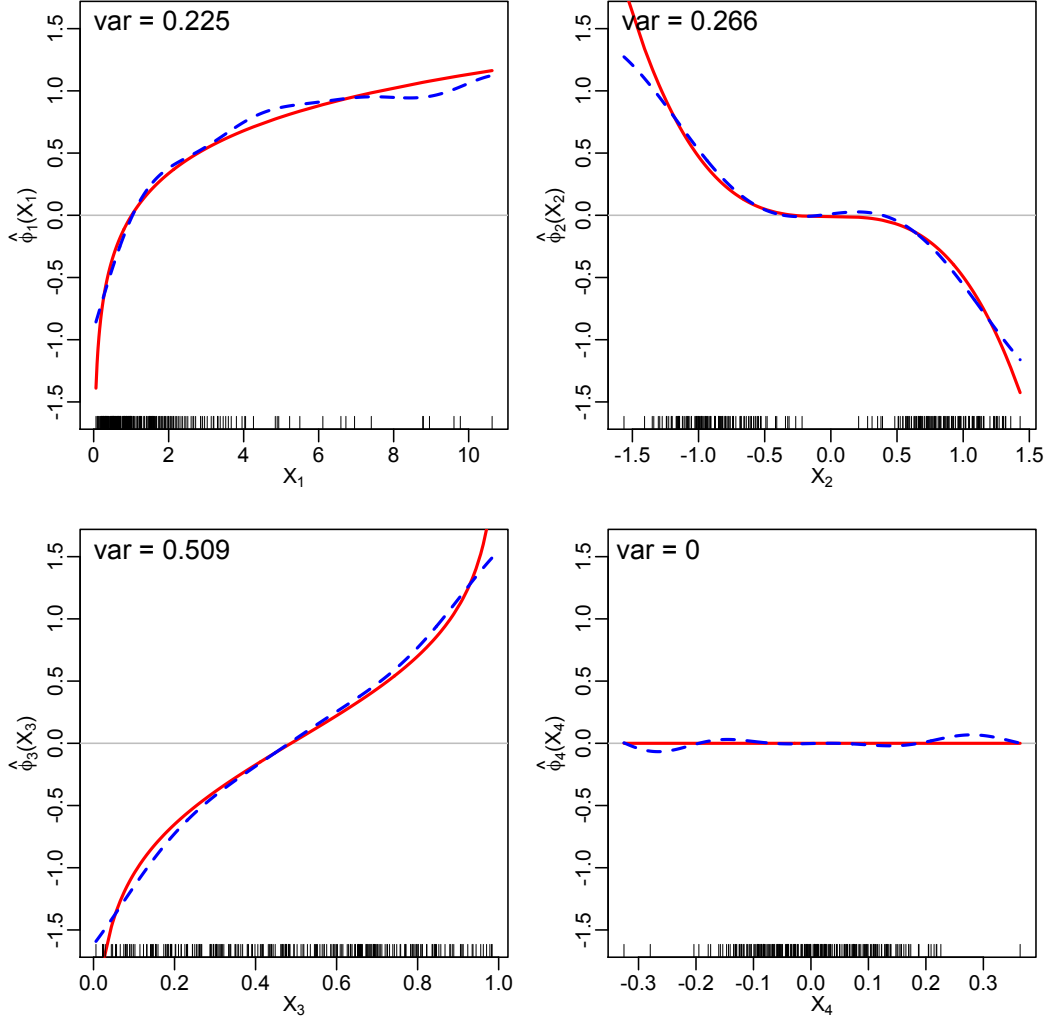


Figure 6: Plot of transformations in population APC (—) and transformations in kernelized sample APC (---). The black bars at the bottom of each plot indicate the location of data points for that variable. The kernelized sample APC is obtained from power algorithm using gaussian kernel for individual variables, with penalty parameters chosen by 5-fold cross-validation. The sample eigenvalue for the estimated APC is 0.0035.

Next, we study the effects that different values of penalty parameters have on the resulting kernelized sample APCs, and we examine the performance of the cross-validation procedure described in Section 3.2. We consider a range of sample sizes  $n \in \{20, 50, 100, 250, 500\}$  and penalty parameters  $\alpha \in \{1.5^{-29}, 1.5^{-28}, \dots, 1.5^5\}$ . For each combination of  $n$  and  $\alpha$ , we compute the true estimation error  $\text{Var} [\hat{\phi}_j(X_j) - \phi_j^*(X_j)]$ , by evaluating  $\hat{\phi}_j$  and  $\phi_j^*$  on  $n = 10,000$  samples generated from the true distribution, for  $1 \leq j \leq 4$ . Figure 7 displays the average estimation error curves

computed from 100 simulated data sets. The crosses denote the locations where  $\alpha$  achieves the minimum estimation error (which can be different from variable to variable), one for each sample size, while the circles represent the average value of the tuning parameters selected by the proposed cross-validation procedure (which is set to be identical for all variables) and its average estimation error. Figure 7 suggests that the proposed cross-validation procedure performs reasonably well when  $n$  is sufficiently large — although it tends to overestimate the optimal tuning parameters, the resulting estimation error is generally close to the best achievable value.

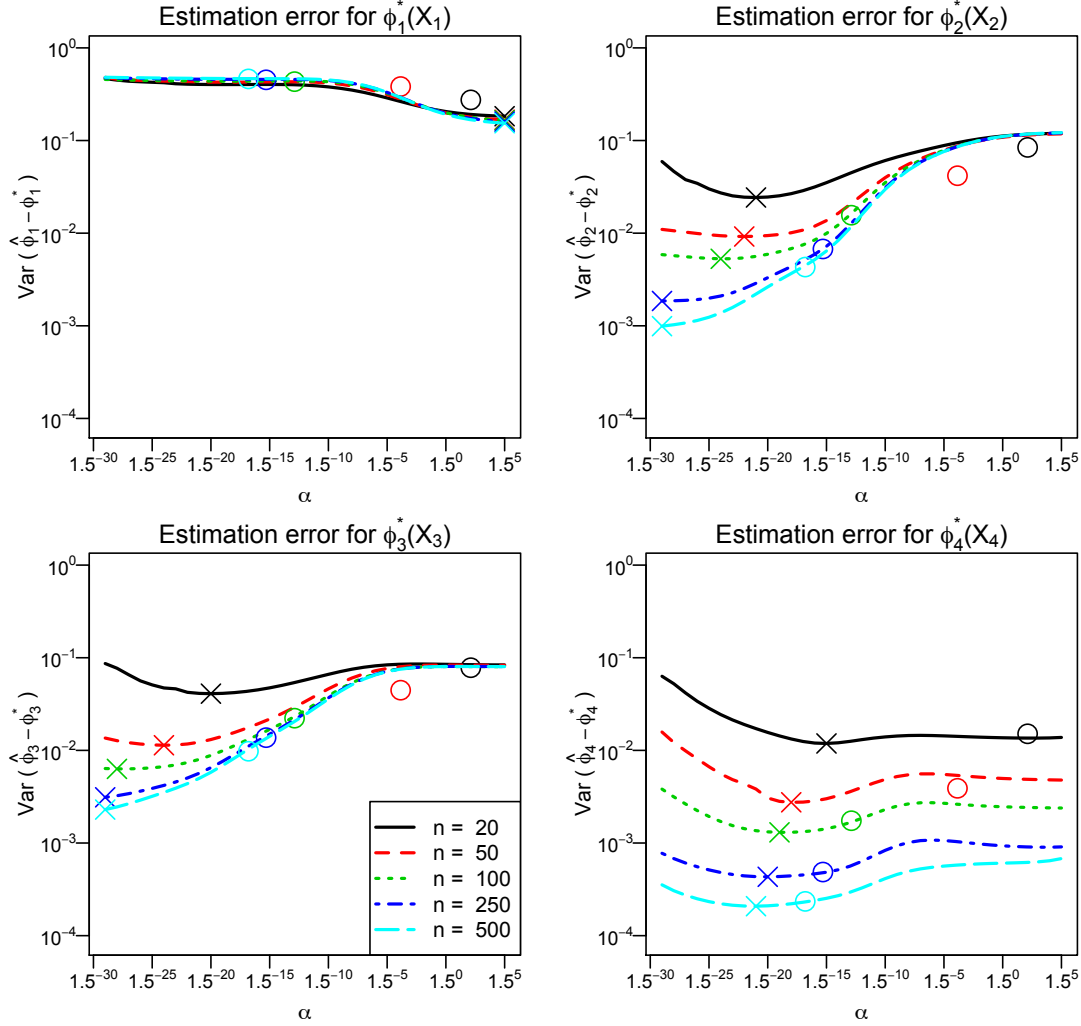


Figure 7: Variance of the difference between the true function  $\phi_j^*$  and its estimate  $\hat{\phi}_j$  obtained from power algorithm using gaussian kernel, for  $1 \leq j \leq 4$ . Crosses: points with lowest estimation error; circles: average penalty parameter values chosen by cross-validation and the average estimation error, the average being taken over 100 simulated data sets.

## 5 Regularization of APCs via Reproducing Kernel Hilbert Spaces

In this section, we formalize the statement of the APC problem in reproducing kernel Hilbert spaces.

### 5.1 Fundamentals of Reproducing Kernel Hilbert Spaces

Let  $\mathcal{X}$  be a nonempty set, and let  $\mathcal{H}$  be a Hilbert space of functions  $f : \mathcal{X} \rightarrow \mathbb{R}$ , endowed with the inner product  $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ . The space  $\mathcal{H}$  is a *reproducing kernel Hilbert space* (RKHS) if all evaluation functionals (the maps  $\delta_x : f \rightarrow f(x)$ , where  $x \in \mathcal{X}$ ) are bounded. Equivalently,  $\mathcal{H}$  is an RKHS if there exists a symmetric function  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  that satisfies (a)  $\forall x \in \mathcal{X}, k_x = k(x, \cdot) \in \mathcal{H}$ , (b) the reproducing property:  $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \langle f, k_x \rangle_{\mathcal{H}} = f(x)$ . We call such a  $k$  the *reproducing kernel* of  $\mathcal{H}$ . There is a one-to-one correspondence between an RKHS  $\mathcal{H}$  and its reproducing kernel  $k$ . Thus, specifying  $k$  is equivalent to specifying  $\mathcal{H}$ , and we will write  $\langle \cdot, \cdot \rangle_k$  for  $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ . Also,  $\|k_x\|_k^2 = k(x, x)$ .

A distinctive characteristic of an RKHS is that each element  $f$  is a function whose values at any  $x \in \mathcal{X}$  is well-defined, whereas an element of a Hilbert space (i.e.  $L^2(\mathcal{X}, dP)$ ) is usually an equivalence class of functions that equal almost everywhere. Such a characteristic of RKHS is crucial as it allows us to evaluate the function  $f$  at each point  $x \in \mathcal{X}$ .

### 5.2 APCs in Reproducing Kernel Hilbert Spaces

We are now ready to define the search space for kernelized APCs. Let  $X_1, \dots, X_p$  be random observations taking values in arbitrary measurable spaces  $\mathcal{X}_1, \dots, \mathcal{X}_p$ . Let  $P_j(dx_j)$  be the marginal probability measure of  $X_j$ , and let  $P_{1:p}(dx_1, \dots, dx_p)$  be the joint probability measure of  $X_1, \dots, X_p$ . We define the search space for kernelized APCs as  $\mathcal{H} = \mathcal{H}_1 \times \dots \times \mathcal{H}_p$ , where the individual transformation  $\phi_j \in \mathcal{H}_j$ , and  $\mathcal{H}_j$  is an RKHS with reproducing kernel  $k_j : \mathcal{X}_j \times \mathcal{X}_j \rightarrow \mathbb{R}$ . We suppose that  $\mathcal{H}_j$  bears the decomposition

$$\mathcal{H}_j = \mathcal{H}_j^0 \oplus \mathcal{H}_j^1, \quad (10)$$

where  $\mathcal{H}_j^0$  is a finite-dimensional linear subspace of  $\mathcal{H}_j$  with basis  $\{q_{1j}, \dots, q_{m_j j}\}$ ,  $m_j = \dim(\mathcal{H}_j^0) < \infty$ , and  $\mathcal{H}_j^1$  is the orthogonal complement of  $\mathcal{H}_j^0$ . We will refer to  $\mathcal{H}_j^0$  as the null space of  $\mathcal{H}_j$ , as it contains the set of functions in  $\mathcal{H}_j$  that we do not wish to “penalize” (to be explained further). With the decomposition (10), the reproducing kernel  $k_j$  can also be uniquely decomposed as  $k_j = k_j^0 + k_j^1$ , where  $k_j^0(x, \cdot) = \mathbf{P}_j^0 k_j(x, \cdot)$ ,  $k_j^1(x, \cdot) = \mathbf{P}_j^1 k_j(x, \cdot)$ , and  $\mathbf{P}_j^0$  and  $\mathbf{P}_j^1$  denotes the orthogonal projection onto  $\mathcal{H}_j^0$  and  $\mathcal{H}_j^1$ , respectively. Furthermore, the inner product  $\langle f, g \rangle_{k_j}$  on  $\mathcal{H}_j$  can be decomposed as

$$\langle f, g \rangle_{k_j} = \langle f^0, g^0 \rangle_{k_j^0} + \langle f^1, g^1 \rangle_{k_j^1}, \quad \forall f, g \in \mathcal{H}_j, \quad (11)$$

where  $f = f^0 + f^1$ ,  $g = g^0 + g^1$ , with  $f^0, g^0 \in \mathcal{H}_j^0$ ,  $f^1, g^1 \in \mathcal{H}_j^1$ , and the decomposition is again unique.

We define the penalty functional  $J_j$  as a squared semi-norm on  $\mathcal{H}_j$ , by letting

$$J_j(f) = \|f^1\|_{k_j^1}^2 = \|\mathbf{P}_j^1 f\|_{k_j^1}^2, \quad \forall f \in \mathcal{H}_j. \quad (12)$$

With slight abuse of notation, we will write  $J_j(f) = \|f\|_{k_j^1}^2$  hereafter. By definition of  $J_j(f)$ , we see that  $f_j^0 = \mathbf{P}_j^0 f_j$  does not play any role in the regularization of APCs. Hence, we can also write  $\mathcal{H}_j^0 = \{f \in \mathcal{H}_j : J_j(f) = 0\}$ , the set of functions in  $\mathcal{H}_j$  that are not “penalized”.

The kernelized APC problem can be stated in the RKHS framework as follows:

$$\min_{\Phi \in \mathcal{H}} \text{Var} \left( \sum_{j=1}^p \phi_j \right) + \sum_{j=1}^p \alpha_j \|\phi_j\|_{k_j^1}^2 \quad \text{subject to} \quad \sum_{j=1}^p \text{Var}(\phi_j) + \sum_{j=1}^p \alpha_j \|\phi_j\|_{k_j^1}^2 = 1, \quad (13)$$

where  $\alpha_j > 0$  is the penalty parameter for  $X_j$ ,  $j = 1, \dots, p$ .

The second-smallest and other higher order kernelized APCs can be obtained as the solution of (13) subject to additional orthogonality constraints

$$\sum_{j=1}^p \text{Cov}(\phi_{\ell,j}, \phi_j) + \sum_{j=1}^p \alpha_j \langle \phi_{\ell,j}, \phi_j \rangle_{k_j^1} = 0, \quad (14)$$

where  $\Phi_\ell = (\phi_{\ell,1}, \dots, \phi_{\ell,p})$  encompasses all the previous kernelized APCs.

**Remark 1.** A canonical example of RKHS with a null space is the Sobolev space of order  $m$ :

$$\mathcal{H} = \{f : [a, b] \rightarrow \mathbb{R} \mid f, f^{(1)}, \dots, f^{(m-1)} \text{ absolutely continuous, } f^{(m)} \in L^2[a, b]\},$$

with  $J(f) := \int_a^b (f^{(m)}(t))^2 dt$ . In this case, the null space  $\mathcal{H}^0 = \text{span}\{1, x, \dots, x^{m-1}\}$ .

**Remark 2.** More generally, one can construct  $\mathcal{H}$  with the decomposition (10) and (11), starting from an RKHS  $\mathcal{H}^1$  with reproducing kernel  $k^1$ . The idea is to augment  $\mathcal{H}^1$  by a finite-dimensional vector space  $\mathcal{H}^0 = \text{span}\{q_1, \dots, q_m\}$ , where  $\{q_1, \dots, q_m\}$  are linearly independent and  $\mathcal{H}^0 \cap \mathcal{H}^1 = \{0\}$ , and then define

$$\mathcal{H} := \{f : f = f^0 + f^1, f^0 \in \mathcal{H}^0, f^1 \in \mathcal{H}^1\}.$$

Since  $\mathcal{H}^0$  is finite-dimensional, any inner product  $\langle \cdot, \cdot \rangle$  that induces a (strict) norm on  $\mathcal{H}^0$  turns it into an RKHS. To see this, first apply the Gram-schmidt procedure on  $\{q_1, \dots, q_m\}$  to obtain an orthonormal basis  $\{r_1, \dots, r_m\}$  of  $\mathcal{H}^0$ . Given  $f^0 = \sum a_i r_i$  and  $g^0 = \sum b_i r_i$ , define  $\langle f^0, g^0 \rangle_{k^0} = \sum a_i b_i$  and  $k^0(x, x') = \sum r_i(x) r_i(x')$ . Then  $\mathcal{H}^0$  is an RKHS with inner product  $\langle \cdot, \cdot \rangle_{k^0} \equiv \langle \cdot, \cdot \rangle$ . By Aronszajn (1950) (page 352-354),  $\mathcal{H}$  as defined is an RKHS with reproducing kernel  $k = k^0 + k^1$ . Note, however, that the reproducing structure of  $\mathcal{H}^0$  actually does not come into play in the kernelized APC problem, since functions in this space go unpenalized.

## 6 Consistency

We define the population APC  $\Phi^* = (\phi_1^*, \dots, \phi_p^*)$ , when it exists, as the solution to

$$\min_{\Phi \in \mathcal{H}} \text{Var} \left( \sum_{j=1}^p \phi_j \right) \quad \text{subject to} \quad \sum_{j=1}^p \text{Var}(\phi_j) = 1. \quad (15)$$

On the other hand, the kernelized sample APC  $\hat{\Phi}^{(n)} = (\hat{\phi}_1^{(n)}, \dots, \hat{\phi}_p^{(n)})$ , when it exists, solves

$$\min_{\Phi \in \mathcal{H}} \widehat{\text{Var}} \left( \sum_{j=1}^p \phi_j \right) + \sum_{j=1}^p \alpha_j \|\phi_j\|_{k_j^1}^2 \quad \text{subject to} \quad \sum_{j=1}^p \widehat{\text{Var}}(\phi_j) + \sum_{j=1}^p \alpha_j \|\phi_j\|_{k_j^1}^2 = 1. \quad (16)$$

The superscript  $(n)$  is to emphasize the dependence of  $\hat{\Phi}^{(n)}$  on the number of observed vectors  $n$ .

In this section, we establish the existence and uniqueness of  $\Phi^*$  and also the consistency of  $\hat{\Phi}^{(n)}$  as an estimator of  $\Phi^*$  under mild conditions.

## 6.1 Preliminaries

Let  $\mathcal{H}, \mathcal{H}_1, \mathcal{H}_2$  be separable Hilbert spaces. We denote the norm of a bounded linear operator  $\mathbf{T}$  by  $\|\mathbf{T}\| := \sup_{\|f\| \leq 1} \|\mathbf{T}f\|$ . The null space and the range of an operator  $\mathbf{T} : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  are denoted by  $\mathcal{N}(\mathbf{T})$  and  $\mathcal{R}(\mathbf{T})$ , respectively, where  $\mathcal{N}(\mathbf{T}) = \{f \in \mathcal{H}_1 : \mathbf{T}f = 0\}$  and  $\mathcal{R}(\mathbf{T}) = \{\mathbf{T}f \in \mathcal{H}_2 : f \in \mathcal{H}_1\}$ . We denote by  $\mathbf{T}^*$  the Hilbert space adjoint of  $\mathbf{T}$ . We say that  $\mathbf{T} : \mathcal{H} \rightarrow \mathcal{H}$  is self-adjoint if  $\mathbf{T}^* = \mathbf{T}$ , and that a bounded linear self-adjoint operator  $\mathbf{T}$  is positive if  $\langle f, \mathbf{T}f \rangle \geq 0$  for all  $f \in \mathcal{H}$ . We write  $\mathbf{T} \succeq 0$  if  $\mathbf{T}$  is positive, and  $\mathbf{T}_1 \succeq \mathbf{T}_2$  if  $\mathbf{T}_1 - \mathbf{T}_2$  is positive. If  $\mathbf{T}$  is positive, we denote by  $\mathbf{T}^{1/2}$  the unique positive operator  $\mathbf{B}$  satisfying  $\mathbf{B}^2 = \mathbf{T}$ . We always denote by  $\mathbf{I}$  the identity operator. A bounded linear operator  $\mathbf{T} : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  is compact if for every bounded sequence  $\{f_n\} \in \mathcal{H}_1$ ,  $\{\mathbf{T}f_n\}$  has a convergent subsequence in  $\mathcal{H}_2$ . For other standard functional analysis concepts such as trace class and Hilbert–Schmidt operators, see [Reed and Simon \(1980\)](#). Finally, we denote by  $[p]$  the set  $\{1, \dots, p\}$ .

## 6.2 Main Assumptions

We now state the main assumptions used to establish the consistency result.

### 6.2.1 Reproducing Kernel Hilbert Spaces

We impose the following assumptions on the kernelized APC search space  $\mathcal{H} = \mathcal{H}_1 \times \dots \times \mathcal{H}_p$ :

**Assumption 1.** For  $1 \leq j \leq p$ , let  $\mathcal{H}_j = \mathcal{H}_j^0 \oplus \mathcal{H}_j^1$  be an RKHS with reproducing kernel  $k_j = k_j^0 + k_j^1$  consisting of real-valued functions with domain  $\mathcal{X}_j$ , where

- (a)  $\mathcal{X}_j$  is a compact metric space;
- (b)  $\mathcal{H}_j^0 \subset C(\mathcal{X}_j)$  with  $\dim(\mathcal{H}_j^0) = m_j < \infty$ ;
- (c)  $k_j^1(x, x')$  is jointly continuous on  $\mathcal{X}_j \times \mathcal{X}_j$ ;
- (d)  $P_j(dx_j)$  is a Borel probability measure fully supported on  $\mathcal{X}_j$ .

The following is an immediate consequence of Assumption 1 (see, e.g., Lemmas 15 and 16).

**Lemma 1.** Under Assumption 1,  $E[k_j(X_j, X_j)] < \sup_{x \in \mathcal{X}_j} k_j(x, x) < \infty$  and  $\mathcal{H}_j \subset C(\mathcal{X}_j) \subset L^2(\mathcal{X}_j, dP_j)$ , for  $1 \leq j \leq p$ .

### 6.2.2 Cross-Covariance Operators

Following [Fukumizu et al. \(2007\)](#), we define the mean element  $m_j \in \mathcal{H}_j$  with respect to a random variable  $X_j$  as

$$\langle \phi_j, m_j \rangle_{k_j} = E[\langle \phi_j, k_{X_j} \rangle_{k_j}] = E[\phi_j(X_j)] \quad \forall \phi_j \in \mathcal{H}_j.$$

On the other hand, we define the cross-covariance operator of  $(X_i, X_j)$  as a bounded linear operator from  $\mathcal{H}_j$  to  $\mathcal{H}_i$  given by

$$\begin{aligned} \langle \phi_i, \mathbf{C}_{ij} \phi_j \rangle_{k_i} &= E[\langle \phi_i, k_{X_i} - m_i \rangle_{k_i} \langle \phi_j, k_{X_j} - m_j \rangle_{k_j}] \\ &= \text{Cov}[\phi_i(X_i), \phi_j(X_j)] \end{aligned} \quad \forall \phi_i \in \mathcal{H}_i, \phi_j \in \mathcal{H}_j.$$

The existence and uniqueness of both  $m_j$  and  $\mathbf{C}_{ij}$  are proved by the Riesz Representation Theorem. It is immediate that  $\mathbf{C}_{ij} = \mathbf{C}_{ji}^*$ . In particular, when  $i = j$ , the self-adjoint operator  $\mathbf{C}_{jj}$  is called the covariance operator. It can be verified that  $\mathbf{C}_{jj}$  is positive and trace-class ([Baker, 1973](#)). Under



Assumption 1,  $\text{Var}[\phi_j(X_j)] = 0$  if and only if  $\phi_j$  is a constant function. Hence, the null space is  $\mathcal{N}(\mathbf{C}_{jj}) = \mathcal{H}_j \cap \mathbb{R}$ .

Let  $\{(X_{\ell 1}, \dots, X_{\ell p}) : 1 \leq \ell \leq n\}$  be i.i.d. random vectors on  $\mathcal{X}_1 \times \dots \times \mathcal{X}_p$  with joint distribution  $P_{1:p}(dx_1, \dots, dx_p)$ . The empirical cross-covariance operator  $\hat{\mathbf{C}}_{ij}^{(n)}$  is defined as the cross-covariance operator with respect to the empirical distribution  $\frac{1}{n} \sum_{\ell=1}^n \delta_{X_{\ell i}} \delta_{X_{\ell j}}$ , in which case

$$\begin{aligned} \langle \phi_i, \hat{\mathbf{C}}_{ij}^{(n)} \phi_j \rangle_{k_i} &= \frac{1}{n} \sum_{\ell=1}^n \left\langle \phi_i, k_{X_{\ell i}} - \frac{1}{n} \sum_{a=1}^n k_{X_{a i}} \right\rangle_{k_i} \left\langle \phi_j, k_{X_{\ell j}} - \frac{1}{n} \sum_{b=1}^n k_{X_{b j}} \right\rangle_{k_j} \\ &= \widehat{\text{Cov}}(\phi_i, \phi_j), \quad \forall \phi_i \in \mathcal{H}_i, \phi_j \in \mathcal{H}_j. \end{aligned}$$

Since  $\mathcal{R}(\hat{\mathbf{C}}_{ij}^{(n)})$  and  $\mathcal{N}(\hat{\mathbf{C}}_{ij}^{(n)})^\perp$  are included in  $\text{span}\{k_{X_{\ell i}} - \frac{1}{n} \sum_{a=1}^n k_{X_{a i}} : 1 \leq \ell \leq n\}$  and  $\text{span}\{k_{X_{\ell j}} - \frac{1}{n} \sum_{b=1}^n k_{X_{b j}} : 1 \leq \ell \leq n\}$ , respectively,  $\hat{\mathbf{C}}_{ij}^{(n)}$  is of finite rank.

It is known (Baker, 1973, Theorem 1) that  $\mathbf{C}_{ij}$  has a representation

$$\mathbf{C}_{ij} = \mathbf{C}_{ii}^{1/2} \mathbf{V}_{ij} \mathbf{C}_{jj}^{1/2}, \quad (17)$$

where  $\mathbf{V}_{ij} : \mathcal{H}_j \rightarrow \mathcal{H}_i$  is a unique bounded linear operator with  $\|\mathbf{V}_{ij}\| \leq 1$ . Moreover,  $\mathbf{V}_{ij} = \mathbf{Q}_i \mathbf{V}_{ij} \mathbf{Q}_j$  where  $\mathbf{Q}_i$  is the orthogonal projection of  $\mathcal{H}_i$  onto  $\overline{\mathcal{R}(\mathbf{C}_{ii})}$ . This implies that  $\mathcal{R}(\mathbf{V}_{ij}) \subseteq \mathcal{R}(\mathbf{C}_{ii})$ .

The following assumption will be used to establish the existence and uniqueness of  $\Phi^*$  in  $\mathcal{H}$ .

**Assumption 2.** The operator  $\mathbf{V}_{ij}$  is compact for  $1 \leq i, j \leq p$ ,  $i \neq j$ . Moreover, the smallest eigenvalue of the operator  $\mathbf{V} - \mathbf{I}$ , where  $\mathbf{V} = (\mathbf{V}_{ij})_{i,j \in [p]}$ ,  $\mathbf{V}_{jj} = \mathbf{I}$  for any  $j \in [p]$ , is simple.

**Remark 3.** The following condition used in Fukumizu et al. (2007, Theorem 3) is sufficient for  $\mathbf{V}_{ij}$  to be Hilbert-Schmidt, which in turn implies compactness: suppose that  $X_i, X_j$  have joint density  $f_{i,j}(x_i, x_j)$  and marginal densities  $f_i(x_i), f_j(x_j)$ , then  $\mathbf{V}_{ij}$  is Hilbert-Schmidt provided

$$\iint \frac{f_{i,j}^2(x_i, x_j)}{f_i(x_i) f_j(x_j)} dx_i dx_j < \infty. \quad (18)$$

Condition (18) is also sufficient to guarantee the existence of population APC  $\Phi^{**}$  in  $\mathbf{H} = H_1 \times \dots \times H_p$ , where  $H_j = L^2(\mathcal{X}_j, dP_j)$ . Under the assumption that  $\mathcal{H}_j$  is dense in  $L^2(\mathcal{X}_j, dP_j)$ , we have  $\Phi^{**} = \Phi^*$ , up to an almost sure constant function.

Due to the presence of the spaces  $\mathcal{H}_j^0$  of unpenalized functions, we need an additional assumption. Noting that  $\mathcal{H}_j = \mathcal{H}_j^0 \oplus \mathcal{H}_j^1$ , we can zoom in on the covariance operator  $\mathbf{C}_{jj}$  and see that it induces the (restricted) covariance operators  $\mathbf{C}_{j0,j0}$  and  $\mathbf{C}_{j1,j1}$  on  $\mathcal{H}_j^0$  and  $\mathcal{H}_j^1$ , and the cross-covariance operator  $\mathbf{C}_{j0,j1} : \mathcal{H}_j^1 \rightarrow \mathcal{H}_j^0$ . Similar as before, by Theorem 1 of Baker (1973),  $\mathbf{C}_{j0,j1}$  has the representation

$$\mathbf{C}_{j0,j1} = \mathbf{C}_{j0,j0}^{1/2} \mathbf{V}_{j0,j1} \mathbf{C}_{j1,j1}^{1/2},$$

where  $\mathbf{V}_{j0,j1} : \mathcal{H}_j^1 \rightarrow \mathcal{H}_j^0$  is a unique bounded linear operator with  $\|\mathbf{V}_{j0,j1}\| \leq 1$ . The following assumption will be used to establish the existence of solutions to a kernelized population APC problem, which is a key step in the proof as we will detail in Section 6.4.

**Assumption 3.** For  $1 \leq j \leq p$ ,  $\mathbf{C}_{j0,j0} \succeq b\mathbf{I}$  and  $\|\mathbf{V}_{j0,j1}\| \leq \sqrt{1 - a/b}$  for some absolute positive constants  $a < b$ .

### 6.3 Statement of Main Theorem

For simplicity, we set the penalty parameters  $\alpha_j$  in the kernelized sample APC problem (16) at a common level  $\epsilon_n$ . The following result establishes the consistency of kernelized sample APCs.

**Theorem 1.** *Suppose that Assumptions 1, 2 and 3 hold, and  $f_j^* \in \mathcal{R}(\mathbf{C}_{jj})$ , for  $1 \leq j \leq p$ . Let  $(\epsilon_n)_{n=1}^\infty$  be a sequence of positive numbers such that*

$$\lim_{n \rightarrow \infty} \epsilon_n = 0, \quad \lim_{n \rightarrow \infty} \frac{n^{-1/3}}{\epsilon_n} = 0. \quad (19)$$

*Then, for any  $\delta > 0$ , there exists  $N(\delta)$  such that for all  $n \geq N(\delta)$ , with probability greater than  $1 - \delta$ , the kernelized sample APC problem (16) has a unique solution  $\hat{\Phi}^{(n)} = (\hat{\phi}_1^{(n)}, \dots, \hat{\phi}_p^{(n)})$  which satisfies*

$$\sum_{j=1}^p \text{Var} [\hat{\phi}_j^{(n)}(X_j) - \phi_j^*(X_j)] < \delta, \quad \text{and} \quad (20)$$

$$|\hat{\lambda}_1^{(n)} - \lambda_1| < \delta, \quad (21)$$

where  $\lambda_1 = \text{Var}(\sum \phi_j^*)$  and  $\hat{\lambda}_1^{(n)} = \widehat{\text{Var}}(\sum \hat{\phi}_j^{(n)}) + \sum \epsilon_n \|\hat{\phi}_j^{(n)}\|_{k_j^1}^2$ .

Note that in (20), for each  $1 \leq j \leq p$ , the variance is taken with respect to the future observation  $X_j$  and the observed data encoded by  $(\hat{\cdot})$  is not integrated out, implying that  $\sum_{j=1}^p \text{Var} [\hat{\phi}_j^{(n)}(X_j) - \phi_j^*(X_j)]$  is a random quantity. In essence, the convergence in (20) says that the difference between the kernelized sample APC and the population APC converges to a constant in probability, while the convergence in (21) says that the optimal value of the kernelized sample criterion converges to the optimal value of the population criterion.

### 6.4 Outline of Proof

In what follows, we lay out the key steps in proving Theorem 1; the detailed arguments are deferred to Appendix A. To study the convergence of  $\hat{\Phi}^{(n)}$  to  $\Phi^*$ , we show that both converge to the kernelized population APC defined as the solution to (13).

#### 6.4.1 Quadratic Forms in RKHS Norm

As a first step in the proof, we rewrite (15), (13) and (16) in terms of quadratic forms with respect to the RKHS norm  $\langle \cdot, \cdot \rangle_k$ . To this end, using the cross-covariance operators introduced in Section 6.2 and setting all  $\alpha_j$  to a common level  $\epsilon_n$ , we can rewrite (15), (13) and (16) as follows:

$$\min_{\Phi \in \mathcal{H}} \langle \Phi, \mathbf{C}\Phi \rangle_k \quad \text{subject to} \quad \langle \Phi, \text{diag}(\mathbf{C})\Phi \rangle_k = 1, \quad (22a)$$

$$\min_{\Phi \in \mathcal{H}} \langle \Phi, (\mathbf{C} + \mathbf{J}^{(n)})\Phi \rangle_k \quad \text{subject to} \quad \langle \Phi, (\text{diag}(\mathbf{C}) + \mathbf{J}^{(n)})\Phi \rangle_k = 1, \quad (22b)$$

$$\min_{\Phi \in \mathcal{H}} \langle \Phi, (\hat{\mathbf{C}}^{(n)} + \mathbf{J}^{(n)})\Phi \rangle_k \quad \text{subject to} \quad \langle \Phi, (\text{diag}(\hat{\mathbf{C}}^{(n)}) + \mathbf{J}^{(n)})\Phi \rangle_k = 1, \quad (22c)$$

where

$$\mathbf{C} = (\mathbf{C}_{ij})_{i,j \in [p]}, \quad \hat{\mathbf{C}}^{(n)} = (\hat{\mathbf{C}}_{ij}^{(n)})_{i,j \in [p]} \quad \text{and} \quad \mathbf{J}^{(n)} = \text{diag}(\epsilon_n \mathbf{P}_j^1)_{j \in [p]},$$

with  $\mathbf{P}_j^1 : \mathcal{H}_j \rightarrow \mathcal{H}_j^1$  the orthogonal projection of  $\mathcal{H}_j$  onto its closed subspace  $\mathcal{H}_j^1$ .

Note that the constraints in (22a) – (22c) are different. To resolve this issue we introduce the following changes of variables:

$$f_j = \mathbf{C}_{jj}^{1/2} \phi_j, \quad (23a)$$

$$f_j = (\mathbf{C}_{jj} + \epsilon_n \mathbf{P}_j^1)^{1/2} \phi_j, \quad (23b)$$

$$f_j = (\hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1)^{1/2} \phi_j, \quad (23c)$$

for  $1 \leq j \leq p$  in (22a) – (22c), respectively. Thus, (22a) – (22c) can be further rewritten as

$$\min_{\mathbf{f} \in \mathcal{H}} \langle \mathbf{f}, \mathbf{V} \mathbf{f} \rangle_k \quad \text{subject to} \quad \langle \mathbf{f}, \mathbf{f} \rangle_k = 1, \quad (24a)$$

$$\min_{\mathbf{f} \in \mathcal{H}} \langle \mathbf{f}, \tilde{\mathbf{V}}^{(n)} \mathbf{f} \rangle_k \quad \text{subject to} \quad \langle \mathbf{f}, \mathbf{f} \rangle_k = 1, \quad (24b)$$

$$\min_{\mathbf{f} \in \mathcal{H}} \langle \mathbf{f}, \hat{\mathbf{V}}^{(n)} \mathbf{f} \rangle_k \quad \text{subject to} \quad \langle \mathbf{f}, \mathbf{f} \rangle_k = 1, \quad (24c)$$

respectively, with

$$\mathbf{V} = (\mathbf{V}_{ij})_{i,j \in [p]}, \quad \tilde{\mathbf{V}}^{(n)} = (\tilde{\mathbf{V}}_{ij}^{(n)})_{i,j \in [p]}, \quad \hat{\mathbf{V}}^{(n)} = (\hat{\mathbf{V}}_{ij}^{(n)})_{i,j \in [p]}, \quad (25)$$

where  $\mathbf{V}_{jj} = \tilde{\mathbf{V}}_{jj}^{(n)} = \hat{\mathbf{V}}_{jj}^{(n)} = \mathbf{I}$  for any  $j \in [p]$  and

$$\mathbf{V}_{ij} = \mathbf{C}_{ii}^{-1/2} \mathbf{C}_{ij} \mathbf{C}_{jj}^{-1/2}, \quad (26a)$$

$$\tilde{\mathbf{V}}_{ij}^{(n)} = (\mathbf{C}_{ii} + \epsilon_n \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ij} (\mathbf{C}_{jj} + \epsilon_n \mathbf{P}_j^1)^{-1/2}, \quad (26b)$$

$$\hat{\mathbf{V}}_{ij}^{(n)} = (\hat{\mathbf{C}}_{ii}^{(n)} + \epsilon_n \mathbf{P}_i^1)^{-1/2} \hat{\mathbf{C}}_{ij}^{(n)} (\hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1)^{-1/2}, \quad (26c)$$

for  $1 \leq i, j \leq p$ ,  $i \neq j$ . By (17),  $\mathbf{V}_{ij}$  is uniquely defined. With slight abuse of notation, we write  $\mathbf{V}_{ij}$  as in (26a) even when  $\mathbf{C}_{ii}^{-1/2}$  and  $\mathbf{C}_{jj}^{-1/2}$  are not appropriately defined as operators. Note, however, that we do need to ensure the operators  $(\mathbf{C}_{jj} + \epsilon_n \mathbf{P}_j^1)^{-1/2}$  and  $(\hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1)^{-1/2}$  in (26b) and (26c) are well-defined with high probability. This is guaranteed by the following lemma, the proof of which is given in Lemmas 10 and 13.

**Lemma 2.** *Under the conditions of Theorem 1, for sufficiently large values of  $n$ ,  $\mathbf{C}_{jj} + \epsilon_n \mathbf{P}_j^1 \succeq \epsilon_n \mathbf{I}$  for  $1 \leq j \leq p$ , and with probability at least  $1 - 2d\epsilon_n^{-1}n^{-1/2}$ ,*

$$\hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1 \succeq \frac{\epsilon_n}{2} \mathbf{I}, \quad \text{for } 1 \leq j \leq p,$$

where  $d$  is a constant not depending on  $n$ .

Next, we show that the solutions to (24a)–(24c) exist. To this end, we are to show that the operators  $\mathbf{V} - \mathbf{I}$ ,  $\tilde{\mathbf{V}}^{(n)} - \mathbf{I}$  and  $\hat{\mathbf{V}}^{(n)} - \mathbf{I}$  are all compact with high probability. Note that for any  $i \neq j$ , the compactness assumption on  $\mathbf{V}_{ij}$  readily shows that  $\mathbf{V} - \mathbf{I}$  is compact. Moreover, using the fact that the product of a bounded linear operator and a compact operator is compact, and that both  $\mathbf{C}_{ii}^{1/2}$  and  $(\mathbf{C}_{ii} + \epsilon_n \mathbf{P}_i^1)^{-1/2}$  are bounded and  $\mathbf{V}_{ij}$  is compact, we see that  $\tilde{\mathbf{V}}_{ij}^{(n)}$  is also compact. Last but not least, on the event that it is well-defined,  $\hat{\mathbf{V}}_{ij}^{(n)}$  is compact since it is of finite-rank. In summary, we have the following result.

**Corollary 1.** *On the event that the conclusions of Lemma 2 hold, under Assumption 2, the operators  $\mathbf{V} - \mathbf{I}$ ,  $\tilde{\mathbf{V}}^{(n)} - \mathbf{I}$  and  $\hat{\mathbf{V}}^{(n)} - \mathbf{I}$  are well-defined and compact.*

Note that compactness implies the spectra of  $\mathbf{V} - \mathbf{I}$ ,  $\tilde{\mathbf{V}}^{(n)} - \mathbf{I}$  and  $\hat{\mathbf{V}}^{(n)} - \mathbf{I}$  are countable with 0 the only possible accumulation point. Consequently, the spectra of  $\mathbf{V}$ ,  $\tilde{\mathbf{V}}^{(n)}$  and  $\hat{\mathbf{V}}^{(n)}$  are countable with +1 as the only possible accumulation point. Assuming that the smallest eigenvalue of  $\mathbf{V}$  has multiplicity one, the solutions to (24a)–(24c) can be obtained as the eigenfunctions  $\mathbf{f}^*$ ,  $\tilde{\mathbf{f}}^{(n)}$  and  $\hat{\mathbf{f}}^{(n)}$  corresponding to the smallest eigenvalues of  $\mathbf{V}$ ,  $\tilde{\mathbf{V}}^{(n)}$  and  $\hat{\mathbf{V}}^{(n)}$ , respectively. In particular,  $\mathbf{f}^*$ ,  $\tilde{\mathbf{f}}^{(n)}$  and  $\hat{\mathbf{f}}^{(n)}$  are unique (with high probability). We can then obtain the solutions to our APC problems by inverse transforming  $\mathbf{f}^*$ ,  $\tilde{\mathbf{f}}^{(n)}$ ,  $\hat{\mathbf{f}}^{(n)}$  following (23a)–(23c). By definition,  $\mathbf{V}$ ,  $\tilde{\mathbf{V}}^{(n)}$  and  $\hat{\mathbf{V}}^{(n)}$  are all positive, so their eigenvalues are bounded below by 0.

In summary, we rewrite the APC problems as in (22a)–(22c) and (24a)–(24c), and we know that under Assumptions 1, 2 and 3, the solutions to (22a)–(22c) and (24a)–(24c) exist.

### 6.4.2 Convergence

We now turn to establishing the consistency of kernelized sample APCs. We start by proving the following two key lemmas, which will lend support to the proof of our main theorems. The first lemma deals with the difference between  $\hat{\mathbf{V}}_{ij}^{(n)}$  and  $\tilde{\mathbf{V}}_{ij}^{(n)}$  which constitutes the stochastic error.

**Lemma 3.** *Under the conditions of Theorem 1, for sufficiently large values of  $n$ , with probability greater than  $1 - 2(d_i + d_j)\epsilon^{-1}n^{-1/2}$ , we have*

$$\|\hat{\mathbf{V}}_{ij}^{(n)} - \tilde{\mathbf{V}}_{ij}^{(n)}\| \leq C\epsilon_n^{-3/2}n^{-1/2}, \quad (27)$$

where  $C$ ,  $d_i$  and  $d_j$  are constants not depending on  $n$ .

The second lemma deals with the *deterministic* difference between  $\tilde{\mathbf{V}}_{ij}^{(n)}$  and  $\mathbf{V}_{ij}$  which can be viewed as approximation error.

**Lemma 4.** *Suppose that Assumptions 1, 2 and 3 hold, and let  $(\epsilon_n)_{n=1}^\infty$  be a sequence of positive numbers such that  $\lim_{n \rightarrow \infty} \epsilon_n = 0$ . Then*

$$\|\tilde{\mathbf{V}}_{ij}^{(n)} - \mathbf{V}_{ij}\| \rightarrow 0 \quad (\text{as } n \rightarrow \infty). \quad (28)$$

Combining Lemma 3 and 4 leads to the following result:

**Theorem 2.** *Suppose that Assumptions 1, 2 and 3 hold, and that the eigenspace which attain the eigenvalue problem*

$$\min_{\mathbf{f} \in \mathcal{H}} \langle \mathbf{f}, \mathbf{V}\mathbf{f} \rangle_k \quad \text{subject to } \langle \mathbf{f}, \mathbf{f} \rangle_k = 1$$

*is one-dimensional, spanned by  $\mathbf{f}^* = (f_1^*, \dots, f_p^*)$  with  $\langle \mathbf{f}^*, \mathbf{f}^* \rangle_k = 1$ . Let  $(\epsilon_n)_{n=1}^\infty$  be a sequence of positive numbers which satisfies (19). Let  $\hat{\mathbf{f}}^{(n)}$  be the unit eigenfunction for the smallest eigenvalue of  $\hat{\mathbf{V}}^{(n)}$ . Then,*

$$|\langle \hat{\mathbf{f}}^{(n)}, \mathbf{f}^* \rangle_k| \rightarrow 1$$

*in probability, as  $n \rightarrow \infty$ .*

Finally, Theorem 1 follows from Theorem 2 once we transform  $\mathbf{f}^*$  and  $\hat{\mathbf{f}}^{(n)}$  back to  $\Phi^*$  and  $\hat{\Phi}^{(n)}$  using the relationship in (23a) and (23c). For details of the proof for the two key lemmas and main theorems, see Appendices A.3 and A.4.

## 7 Estimation and Computation

In this section, we motivate an iterative method for computing kernelized APCs. This involves the use of power algorithm, an iterative algorithm for extracting the first few largest (or smallest) eigenfunctions of a bounded linear operator. In addition to detailing out the algorithm, we provide rigorous theoretical justification of the use of power algorithm in the RKHS framework.

Consider a matrix  $\mathbf{M}$  with the eigen-decomposition  $\mathbf{M} = \sum_{i=1}^m \lambda_i \mathbf{M}_i$ , where  $\mathbf{M}_i = \mathbf{u}_i \mathbf{u}_i^T$  and the eigenvalues  $\lambda_1 > \lambda_2 > \dots > \lambda_m$  are distinct. The power algorithm allows us to compute the eigenvector  $\mathbf{u}_1$  corresponding to the largest eigenvalue  $\lambda_1$  (see, e.g., [Golub and Van Loan \(2013\)](#)) by forming normalized powers  $\mathbf{M}^n \mathbf{u}_0 / \|\mathbf{M}^n \mathbf{u}_0\|$  which can be shown to converge to  $\mathbf{u}_1$  as long as  $\mathbf{u}_0$  is not orthogonal to  $\mathbf{u}_1$ .

To compute the eigenvector  $\mathbf{u}_m$  corresponding to the smallest eigenvalue  $\lambda_m$ , the spectrum needs to be flipped and shifted by replacing  $\mathbf{M}$  with  $\gamma \mathbf{I} - \mathbf{M}$  in the power algorithm. If  $0 \leq \lambda_1 < \lambda_m \leq B$  for some  $B > 0$ , then using  $\gamma = (B + 1)/2$ , we have

$$\begin{aligned} -\frac{B-1}{2} \leq \gamma - \lambda_i &\leq \frac{B-1}{2} && \text{if } 1 \leq \lambda_i \leq B, \\ \frac{B-1}{2} \leq \gamma - \lambda_i &\leq \frac{B-1}{2} + 1 && \text{if } 0 \leq \lambda_i \leq 1. \end{aligned}$$

In this case, the large eigenvalues of  $\mathbf{M}$ ,  $\{\lambda : \lambda > 1\}$ , are mapped to an interval centered at 0, while the small eigenvalues  $\{\lambda : \lambda < 1\}$  are affixed to the right end of this interval.

### 7.1 Eigencharacterization of Kernelized APCs

To relate power algorithm to kernelized APCs, we first show that the kernelized APC problem (13) can be reformulated as an eigenvalue problem with respect to a new inner product  $\langle \cdot, \cdot \rangle_\star$  defined on  $\mathcal{H}$  (which is initially endowed with  $\langle \cdot, \cdot \rangle_k$ ). As a consequence, kernelized APC can be obtained as the eigenfunction corresponding to the smallest eigenvalue of an operator  $\tilde{\mathbf{S}}$  defined on  $(\mathcal{H}, \langle \cdot, \cdot \rangle_\star)$ . Then, computation of kernelized sample APC reduces to an application of power algorithm on an empirical version of  $\tilde{\mathbf{S}}$ .

**Theorem 3.** *Suppose that Assumption 1 holds, and  $\mathcal{H}_j^0$  excludes constants. Then  $\mathcal{H}_j$  is a reproducing kernel Hilbert space with respect to the inner product*

$$\langle f, g \rangle_{\star_j} := \text{Cov}[f(X_j), g(X_j)] + \alpha_j \langle f, g \rangle_{k_j^1}, \quad f, g \in \mathcal{H}_j, \alpha_j > 0.$$

From Theorem 3, we see that it is reasonable to endow  $\mathcal{H} = \mathcal{H}_1 \times \dots \times \mathcal{H}_p$  with the new inner product

$$\langle \Phi, \Psi \rangle_\star := \sum_{j=1}^p \langle \phi_j, \psi_j \rangle_{\star_j},$$

where  $\Phi = (\phi_1, \dots, \phi_p)$ ,  $\Psi = (\psi_1, \dots, \psi_p)$  are both elements of  $\mathcal{H}$ .

We now introduce the smoothing operator  $\mathbf{S}_{ij}$ , defined through a “generalized” regularized population regression problem:

$$\begin{aligned} \mathbf{S}_{ij} : (\mathcal{H}_j, \langle \cdot, \cdot \rangle_{\star_j}) &\longrightarrow (\mathcal{H}_i, \langle \cdot, \cdot \rangle_{\star_i}), \\ \phi_j &\longmapsto \underset{f \in \mathcal{H}_i}{\operatorname{argmin}} \left\{ \text{Var}[\phi_j(X_j) - f(X_i)] + \alpha_i \|f\|_{k_i^1}^2 \right\}. \end{aligned} \tag{29}$$

Indeed, the problem reduces to the population version of the usual regularized regression problem, when  $\phi_j$  and  $f$  are both required to have mean zero. With the establishment of existence and uniqueness of solution to the problem, the smoothing operator  $\mathbf{S}_{ij}$  in (29) mapping  $\phi_j$  to its “smoothed” version in  $\mathcal{H}_i$  is well-defined. In addition, it enjoys some nice properties:

**Theorem 4.** *Suppose that  $(\mathcal{H}_j, \langle \cdot, \cdot \rangle_{k_j})$  is a reproducing kernel Hilbert space satisfying Assumption 1 with  $\mathcal{H}_j^0$  excluding constants, and  $\alpha_j > 0$ , for  $1 \leq j \leq p$ . Then  $\mathbf{S}_{ij}$  is well-defined, bounded, linear, compact, and*

$$\langle \phi_i, \mathbf{S}_{ij} \phi_j \rangle_{\star_i} = \text{Cov}[\phi_i(X_i), \phi_j(X_j)], \quad \forall \phi_i \in \mathcal{H}_i, \phi_j \in \mathcal{H}_j. \quad (30)$$

Moreover,

$$\|\mathbf{S}_{ij} \phi_j\|_{\star_i} \leq (\text{Var}[\phi_j(X_j)])^{1/2} \leq \|\phi_j\|_{\star_j}, \quad \forall \phi_j \in \mathcal{H}_j. \quad (31)$$

Theorem 4 says that the operator  $\mathbf{S}_{ij}$  is not only well-defined, but acts as the “covariance operator” with respect to  $\langle \cdot, \cdot \rangle_{\star_i}$  (whereas the covariance operator  $\mathbf{C}_{ij}$  in Section 6 is defined with respect to  $\langle \cdot, \cdot \rangle_{k_i}$ ). In addition, it is a contraction operation by (31). We are now ready to restate the kernelized APC problem as an eigenvalue problem with respect to the inner product  $\langle \cdot, \cdot \rangle_{\star}$ .

**Theorem 5.** *Let  $\mathcal{H} = \mathcal{H}_1 \times \cdots \times \mathcal{H}_p$ , where  $\mathcal{H}_j$  is a reproducing kernel Hilbert space with respect to  $\langle \cdot, \cdot \rangle_{\star_j}$ , for  $1 \leq j \leq p$ . Then the kernelized APC problem (13) can be restated as*

$$\min_{\Phi \in \mathcal{H}} \langle \Phi, \tilde{\mathbf{S}} \Phi \rangle_{\star} \quad \text{subject to} \quad \langle \Phi, \Phi \rangle_{\star} = 1, \quad (32)$$

where  $\tilde{\mathbf{S}} : \mathcal{H} \rightarrow \mathcal{H}$  is defined by the component mapping

$$[\tilde{\mathbf{S}} \Phi]_i = \sum_{j \neq i} \mathbf{S}_{ij} \phi_j + \phi_i, \quad (33)$$

and  $\mathbf{S}_{ij}$  is the smoothing operator as defined in (29). Moreover,  $\tilde{\mathbf{S}}$  is self-adjoint, positive, and bounded above by  $p$ .

We see that the smoothing operators  $\mathbf{S}_{ij}$ ’s play an important role in the kernelized APC problem. This is reminiscent of the role of orthogonal projection operators  $\mathbf{P}_{ij}$ ’s in the original APC problem in Donnell et al. (1994).

To address the issue of existence of eigenvalues, and hence the solution of (32) when  $\mathcal{H}$  is infinite-dimensional, we recall the usual compactness condition. We know that  $\mathbf{S}_{ij}$  is compact from Theorem 4. Although this does not imply the compactness of  $\tilde{\mathbf{S}}$ , we have the following result:

**Theorem 6.** *The operator  $\tilde{\mathbf{S}} - \mathbf{I} : (\mathcal{H}, \langle \cdot, \cdot \rangle_{\star}) \rightarrow (\mathcal{H}, \langle \cdot, \cdot \rangle_{\star})$ ,*

$$\tilde{\mathbf{S}} - \mathbf{I} = \begin{pmatrix} \mathbf{0} & \mathbf{S}_{12} & \cdots & \mathbf{S}_{1p} \\ \mathbf{S}_{21} & \mathbf{0} & \cdots & \mathbf{S}_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{S}_{p1} & \mathbf{S}_{p2} & \cdots & \mathbf{0} \end{pmatrix},$$

where  $\mathbf{S}_{ij} : (\mathcal{H}_j, \langle \cdot, \cdot \rangle_{\star_j}) \rightarrow (\mathcal{H}_i, \langle \cdot, \cdot \rangle_{\star_i})$  is as given in (29), is compact.

The compactness attribute implies that  $\tilde{\mathbf{S}} - \mathbf{I}$  has an eigendecomposition with eigenvalues that can only accumulate at 0, which in turn implies that the only possible accumulation point of the eigenvalues of  $\tilde{\mathbf{S}}$  is +1. To this end, we see that kernelized APC can be obtained as the eigenfunction corresponding to the smallest eigenvalue of  $\tilde{\mathbf{S}}$ . In addition, we see that +1 is a natural dividing line between smallest and largest kernelized APCs.



## 7.2 Power Algorithm for Kernelized APCs

Applying the knowledge that kernelized APCs are the eigenfunctions of  $\tilde{\mathbf{S}}$  from a population standpoint, we execute the power algorithm on  $\gamma\mathbf{I} - \tilde{\mathbf{S}}$  to solve for the (smallest) kernelized APC. The pseudocode is given below. Here  $\gamma$  is taken to be  $(p+1)/2$  since the spectrum of  $\tilde{\mathbf{S}}$  is bounded above by  $p$ , as claimed in Theorem 5. We see that solving for kernelized APC reduces to iterative smoothing of each component  $\phi_j$  against  $X_i$ , for  $j \neq i$ .

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**Algorithm 1** Computation of kernelized APC

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Let  $\gamma = (p+1)/2$ . Initialize  $t = 0$ ,  $\Phi^{[0]} = (\phi_1^{[0]}, \phi_2^{[0]}, \dots, \phi_p^{[0]})$ .
repeat
  for  $i = 1, \dots, p$  do
     $\phi_i \leftarrow \gamma\phi_i^{[t]} - (\sum_{j \neq i} \mathbf{S}_{ij}\phi_j^{[t]} + \phi_i^{[t]})$  {Update steps}
  end for
  Standardize with  $c = (\sum \|\phi_i\|_{\star_i}^2)^{-1/2}$ 
   $(\phi_1^{[t+1]}, \phi_2^{[t+1]}, \dots, \phi_p^{[t+1]}) \leftarrow (c\phi_1, c\phi_2, \dots, c\phi_p)$ 
   $t \leftarrow t + 1$ 
until  $\text{Var} \sum \phi_i^{[t]} + \sum \alpha_i \|\phi_i^{[t]}\|_{k_i^1}^2$  converges

```

---

To compute the  $k^{\text{th}}$  smallest kernelized APCs for  $k > 1$ , we just need to add a series of Gram-Schmidt steps

$$\phi_i \leftarrow \phi_i - \left( \sum_{j=1}^p \langle \phi_{\ell,j}, \phi_j^{[t]} \rangle_{\star_j} \right) \phi_{\ell,i}, \quad 1 \leq \ell \leq k-1$$

following the update steps in Algorithm 1, to ensure that the orthogonality requirements (14) are satisfied. Here  $\Phi_\ell = (\phi_{\ell,1}, \dots, \phi_{\ell,p})$  is the previously obtained  $\ell^{\text{th}}$  smallest kernelized APC, where  $1 \leq \ell \leq k-1$ .

The power algorithm is guaranteed to converge under mild conditions:

**Proposition 1.** *Suppose that the smallest eigenvalue of  $\tilde{\mathbf{S}}$  is of multiplicity one with corresponding unit eigenfunction  $\tilde{\Phi}$ . If the power algorithm is initialized with  $\Phi^{[0]}$  that has a nontrivial projection onto  $\tilde{\Phi}$ , then the power algorithm converges.*

For implementation details see Appendix C.

## 8 Concluding Remarks

APCs are a useful tool for exploring additive degeneracy in data. In this paper, we propose the estimation of APCs using the shrinkage regularization approach through kernelizing, and we establish the consistency of the resulting kernelized sample APCs.

It would be interesting to generalize our study of APCs in several directions. Due to the nonparametric nature of APC estimation, so far we have implicitly assumed that the sample size  $n$  is large relative to the total number of variables  $p$ . It would be interesting to extend APCs to the high-dimensional setting where  $p$  can be comparable to  $n$ . It would then be natural to impose additional structure such as sparsity in a flavor similar to the sparse additive models proposed by Ravikumar et al. (2009) in the regression framework. It would also be interesting to study the largest APCs and to examine whether it provides meaningful interpretation through dimensionality reduction as in conventional PCA.

Estimation of APCs is non-trivial due to its unsupervised learning nature. We have left open the problems of kernel choice and how to optimally and differentially select smoothing parameters for different variables within an APC and also across different APCs.

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## References

- Aronszajn, N. (1950). Theory of reproducing kernels. *Trans. Amer. Math. Soc.* 68, 337–404.
- Bach, F. R. and M. I. Jordan (2003). Kernel independent component analysis. *J. Mach. Learn. Res.* 3(1), 1–48.
- Baker, C. R. (1973). Joint measures and cross-covariance operators. *Trans. Amer. Math. Soc.* 186, 273–289.
- Breiman, L. and J. H. Friedman (1985). Estimating optimal transformations for multiple regression and correlation. *J. Amer. Statist. Assoc.* 80(391), 580–619. With discussion and with a reply by the authors.
- Buja, A., T. J. Hastie, and R. J. Tibshirani (1989). Linear smoothers and additive models. *Ann. Statist.* 17(2), 453–520. With discussions by Breiman, Chen/Gu/Wahba, D.D.Cox, Eubank/Speckman, Gander/Golub, Gasser/Kneip, Kohn/Ansley, Titterton, and a rejoinder by the authors.
- Cardoso-Cachopo, A. (2009). “<http://web.ist.utl.pt/acardoso/datasets/>”.
- Donnell, D. J., A. Buja, and W. Stuetzle (1994). Analysis of additive dependencies and concavities using smallest additive principal components. *Ann. Statist.* 22(4), 1635–1673. With a discussion by Bernard D. Flury [Bernhard Flury] and a rejoinder by the authors.
- Fukumizu, K., F. R. Bach, and A. Gretton (2007). Statistical consistency of kernel canonical correlation analysis. *J. Mach. Learn. Res.* 8, 361–383.
- Golub, G. H. and C. F. Van Loan (2013). *Matrix computations* (Fourth ed.). Johns Hopkins Studies in the Mathematical Sciences. Johns Hopkins University Press, Baltimore, MD.
- Guo, J., E. Levina, G. Michailidis, and J. Zhu (2011). Joint estimation of multiple graphical models. *Biometrika* 98(1), 1–15.
- Hastie, T. J. and R. J. Tibshirani (1990). *Generalized Additive Models* (Reprint 1999 ed.). Monographs on Statistics and Applied Probability 43. Boca Raton: Chapman & Hall / CRC.
- Jolliffe, I. T. (2002). *Principal component analysis* (Second ed.). Springer Series in Statistics. New York: Springer-Verlag.
- Leurgans, S. E., R. A. Moyeed, and B. W. Silverman (1993). Canonical correlation analysis when the data are curves. *J. Roy. Statist. Soc. Ser. B* 55(3), 725–740.

- Ravikumar, P., J. Lafferty, H. Liu, and L. Wasserman (2009). Sparse additive models. *J. Roy. Statist. Soc. Ser. B Stat. Methodol.* 71(5), 1009–1030.
- Reed, M. and B. Simon (1980). *Methods of modern mathematical physics. I* (Second ed.). New York: Academic Press Inc. [Harcourt Brace Jovanovich Publishers]. Functional analysis.
- Rice, J. A. and B. W. Silverman (1991). Estimating the mean and covariance structure nonparametrically when the data are curves. *J. Roy. Statist. Soc. Ser. B* 53(1), 233–243.
- Schmitt, B. A. (1992). Perturbation bounds for matrix square roots and Pythagorean sums. *Linear Algebra Appl.* 174, 215–227.
- Schölkopf, B. and A. J. Smola (2002). *Learning with kernels: Support Vector Machines, Regularization, Optimization, and Beyond* (First ed.). Cambridge, Massachusetts; London, England: MIT Press.
- Schölkopf, B., A. J. Smola, and K.-R. Müller (1998). Nonlinear component analysis as a kernel eigenvalue problem. *Neural Comp.* 10(3), 1299–1319.
- Silverman, B. W. (1996). Smoothed functional principal components analysis by choice of norm. *Ann. Statist.* 24(1), 1–24.
- Tan, K. M., D. Witten, and A. Shojaie (2015). The cluster graphical lasso for improved estimation of Gaussian graphical models. *Comput. Statist. Data Anal.* 85, 23–36.
- Wahba, G. (1990). *Spline models for observational data*, Volume 59 of *CBMS-NSF Regional Conference Series in Applied Mathematics*. Philadelphia, PA: Society for Industrial and Applied Mathematics (SIAM).

## A Consistency Proof of Section 6

In this section, we give the consistency proof for kernelized sample APCs. We first consider some useful facts from functional analysis in Section A.1. We then present in Section A.2 some basic properties of the operator  $\mathbf{C}_{jj} + \epsilon_n \mathbf{P}_j^1$  and the square root of its inverse (which exists under mild conditions), which forms the building blocks of the proof of two key lemmas and main theorems in Section A.3 and Section A.4.

### A.1 Some Facts from Functional Analysis

**Lemma 5.** *Let  $A, B$  be positive, self-adjoint operators on a Hilbert space. Then*

$$\|A^{1/2} - B^{1/2}\| \leq \frac{\|A - B\|}{\lambda_{\min}(A^{1/2}) + \lambda_{\min}(B^{1/2})}.$$

*Proof.* The proof essentially follows from Schmitt (1992). Let  $D = B - A$  and  $X = B^{1/2} - A^{1/2}$ . It is straightforward to verify that

$$XA^{1/2} + B^{1/2}X = D.$$

It then follows that

$$X = E_2 X E_1 + F, \tag{34}$$

where

$$\begin{aligned} E_1 &= (qI + A^{1/2})^{-1}(qI - A^{1/2}), \\ E_2 &= (qI + B^{1/2})^{-1}(qI - B^{1/2}), \\ F &= 2q(qI + B^{1/2})^{-1}D(qI + A^{1/2})^{-1}, \end{aligned}$$

for all  $q > 0$ . Applying triangle inequality to (34) gives

$$\|X\| \leq \|E_2\| \|X\| \|E_1\| + \|F\|,$$

or, equivalently,

$$\|X\| \leq \frac{\|F\|}{1 - \|E_1\| \|E_2\|}. \tag{35}$$

Our goal now is to find upper bounds for  $\|E_1\| \|E_2\|$  and  $\|F\|$ . An upper bound for  $\|F\|$  is given by

$$\begin{aligned} \|F\| &\leq 2q \|D\| \|(qI + A^{1/2})^{-1}\| \|(qI + B^{1/2})^{-1}\| \\ &\leq \frac{2q \|D\|}{[q + \lambda_{\min}(A^{1/2})][q + \lambda_{\min}(B^{1/2})]}. \end{aligned} \tag{36}$$

We now get an upper bound for  $\|E_1\|^2$ . First note that

$$\begin{aligned} \frac{\|E_1 x\|^2}{\|x\|^2} &= \frac{\|(qI + A^{1/2})^{-1}(qI - A^{1/2})x\|^2}{\|x\|^2}, \quad \text{let } y = (qI + A^{1/2})^{-1}x \\ &= \frac{\|(qI + A^{1/2})^{-1}(qI - A^{1/2})(qI + A^{1/2})y\|^2}{\|(qI + A^{1/2})y\|^2} \\ &= \frac{\|(qI - A^{1/2})y\|^2}{\|(qI + A^{1/2})y\|^2} \\ &= \frac{q^2 \|y\|^2 - 2q \langle y, A^{1/2} y \rangle + \|A^{1/2} y\|^2}{q^2 \|y\|^2 + 2q \langle y, A^{1/2} y \rangle + \|A^{1/2} y\|^2}, \end{aligned}$$

where the third equality is due to commutativity between  $qI - A^{1/2}$  and  $qI + A^{1/2}$ . It then follows that

$$\begin{aligned}
\|E_1\|^2 &= \max_{x \neq 0} \frac{\|E_1 x\|^2}{\|x\|^2} \\
&= \max_{y \neq 0} \frac{q^2 \|y\|^2 - 2q \langle y, A^{1/2} y \rangle + \|A^{1/2} y\|^2}{q^2 \|y\|^2 + 2q \langle y, A^{1/2} y \rangle + \|A^{1/2} y\|^2} \\
&\leq \max_{y \neq 0} \frac{q^2 - 2q \lambda_{\min}(A^{1/2}) + \|A^{1/2} y\|^2 / \|y\|^2}{q^2 + 2q \lambda_{\min}(A^{1/2}) + \|A^{1/2} y\|^2 / \|y\|^2} \\
&= \max_{y \neq 0} \left[ 1 - \frac{4q \lambda_{\min}(A^{1/2})}{q^2 + 2q \lambda_{\min}(A^{1/2}) + \|A^{1/2} y\|^2 / \|y\|^2} \right] \\
&= 1 - \frac{4q \lambda_{\min}(A^{1/2})}{q^2 + 2q \lambda_{\min}(A^{1/2}) + \lambda_{\max}^2(A^{1/2})} \\
&= 1 - \frac{4 \lambda_{\min}(A^{1/2})}{q} + O\left(\frac{1}{q^2}\right), \tag{37}
\end{aligned}$$

the inequality holds because the rational expression is monotonically decreasing in  $\langle y, A^{1/2} y \rangle$ . Similarly, an upper bound for  $\|E_2\|^2$  is

$$\|E_2\|^2 \leq 1 - \frac{4 \lambda_{\min}(B^{1/2})}{q} + O\left(\frac{1}{q^2}\right). \tag{38}$$

So we see that  $\|E_1\| \|E_2\| < 1$  when  $q$  is sufficiently large. Combining (35), (36), (37) and (38) gives

$$\begin{aligned}
\|X\| &\leq \frac{\|F\|}{1 - \|E_1\| \|E_2\|} \leq \frac{\|F\|}{1 - \frac{1}{2}(\|E_1\|^2 + \|E_2\|^2)} \\
&\leq \frac{2q \|D\|}{[q + \lambda_{\min}(A^{1/2})][q + \lambda_{\min}(B^{1/2})]} \cdot \frac{1}{2q^{-1}[\lambda_{\min}(A^{1/2}) + \lambda_{\min}(B^{1/2}) + O(q^{-1})]} \\
&\leq \frac{\|D\|}{\lambda_{\min}(A^{1/2}) + \lambda_{\min}(B^{1/2}) + O(q^{-1})}.
\end{aligned}$$

Sending  $q$  to infinity gives the desired bound.  $\square$

The following lemmas are from Appendix B of [Fukumizu et al. \(2007\)](#), and correspond to Lemma 8 and 9 in [Fukumizu et al. \(2007\)](#), respectively.

**Lemma 6.** *Let  $A$  and  $B$  be positive, self-adjoint operators on a Hilbert space, with  $0 \preceq A \preceq \lambda \mathbf{I}$  and  $0 \preceq B \preceq \lambda \mathbf{I}$  for some  $\lambda > 0$ . Then*

$$\|A^{3/2} - B^{3/2}\| \leq 3\lambda^{1/2} \|A - B\|.$$

**Lemma 7.** *Let  $\mathcal{H}_1, \mathcal{H}_2$  be Hilbert spaces, and let  $\mathcal{H}$  be a dense linear subspace of  $\mathcal{H}_2$ . Suppose that  $A_n$  and  $A$  are bounded operators on  $\mathcal{H}_2$ , and  $B : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  is compact. If*

$$A_n x \rightarrow Ax$$

*for all  $x \in \mathcal{H}$ , and*

$$\sup_n \|A_n\| < \infty,$$

*then  $\|A_n B - AB\| \rightarrow 0$ .*

The following lemma is adapted from Lemma 10 of [Fukumizu et al. \(2007\)](#), but proved for the case of the smallest eigenfunction (rather than the largest eigenfunction).

**Lemma 8.** *Let  $A$  be a compact operator on a Hilbert space  $\mathcal{H}$ , and  $A_n (n \in \mathbb{N})$  be bounded operators on  $\mathcal{H}$  such that  $A_n$  converges to  $A$  in norm. Assume that the eigenspace of  $A$  corresponding to the smallest eigenvalue is one-dimensional and spanned by a unit function  $f_1$ , and the minimum of the spectrum of  $A_n$  is attained by a unit eigenfunction  $\hat{f}_1^{(n)}$ . Then*

$$|\langle \hat{f}_1^{(n)}, f_1 \rangle| \longrightarrow 1 \quad \text{as } n \longrightarrow \infty.$$

*Proof.* Since  $A$  is compact, the eigendecomposition

$$A = \sum_{i=1}^{\infty} \lambda_i \langle f_i, \cdot \rangle f_i$$

holds, where  $\{\lambda_i\}$  is the eigenvalues and  $\{f_i\}$  is the corresponding eigenfunctions so that  $\{f_i\}$  forms a complete orthonormal basis system of  $\mathcal{H}$ . For convenience, we denote by  $\lambda_1$  and  $\lambda_2$  the smallest and second smallest eigenvalue of  $A$ , respectively. By assumption  $\lambda_1 < \lambda_2$ .

Let  $\delta_n = |\langle \hat{f}_1^{(n)}, f_1 \rangle|$ . We have

$$\begin{aligned} \langle \hat{f}_1^{(n)}, A \hat{f}_1^{(n)} \rangle &= \lambda_1 \langle \hat{f}_1^{(n)}, f_1 \rangle^2 + \sum_{i=2}^{\infty} \lambda_i \langle \hat{f}_1^{(n)}, f_i \rangle^2 \\ &\geq \lambda_1 \langle \hat{f}_1^{(n)}, f_1 \rangle^2 + \lambda_2 \sum_{i=2}^{\infty} \langle \hat{f}_1^{(n)}, f_i \rangle^2 \\ &= \lambda_1 \delta_n^2 + \lambda_2 (1 - \delta_n^2) \\ &\geq \lambda_1. \end{aligned} \tag{39}$$

On the other hand, since  $A_n$  converges to  $A$  in norm, we have

$$\sup_{\|f\| \leq 1} \|A_n f - A f\| \longrightarrow 0,$$

hence

$$\sup_{\|f\| \leq 1} \|\langle f, A_n f \rangle - \langle f, A f \rangle\| \leq \sup_{\|f\| \leq 1} \|A_n f - A f\| \longrightarrow 0.$$

This in turn implies that

$$\lambda_1 = \langle f_1, A f_1 \rangle \leq \langle \hat{f}_1^{(n)}, A \hat{f}_1^{(n)} \rangle = \langle \hat{f}_1^{(n)}, A_n \hat{f}_1^{(n)} \rangle + o(1) = \hat{\lambda}_1^{(n)} + o(1), \tag{40}$$

and

$$\hat{\lambda}_1^{(n)} = \langle \hat{f}_1^{(n)}, A_n \hat{f}_1^{(n)} \rangle \leq \langle f_1, A_n f_1 \rangle = \langle f_1, A f_1 \rangle + o(1) = \lambda_1 + o(1). \tag{41}$$

Combining (40) and (41) gives

$$\hat{\lambda}_1^{(n)} \longrightarrow \lambda_1,$$

and it follows that  $\langle \hat{f}_1^{(n)}, A \hat{f}_1^{(n)} \rangle$  must converge to  $\lambda_1$ . Applying this and  $\lambda_1 < \lambda_2$  to (39) gives  $\delta_n^2 \longrightarrow 1$ .  $\square$



## A.2 Proofs of Supporting Lemmas

In this subsection, we will consider some lemmas that will be directly useful for establishing the proofs in Sections A.3 and A.4. The following lemma corresponds to Lemma 5 in Fukumizu et al. (2007), and bounds the Hilbert-Schmidt norm of the difference between the empirical covariance operator and the (population) covariance operator.

**Lemma 9.** *The cross-covariance operator  $\mathbf{C}_{ij}$  is Hilbert-Schmidt, and*

$$E\|\hat{\mathbf{C}}_{ij}^{(n)} - \mathbf{C}_{ij}\|_{HS} = O(n^{-1/2}),$$

where  $\|\cdot\|_{HS}$  denotes the Hilbert-Schmidt norm of a Hilbert-Schmidt operator.

In the following, we first consider a sufficient condition for the operator  $\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1$  to be bounded below by  $\epsilon$ . Once this is done,  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}$  is well-defined and is bounded above by  $\epsilon^{-1/2}$ . To simplify notation, the subscript  $j$  is omitted.

Let  $\mathcal{H} = \mathcal{H}^0 \oplus \mathcal{H}^1$  be an RKHS with reproducing kernel  $k = k^0 + k^1$ . Suppose that each  $f \in \mathcal{H}$  is a real-valued function with domain  $\mathcal{X}$ , and the random variable  $X$  also takes value in  $\mathcal{X}$ . Following Baker (1973) and Fukumizu et al. (2007), under the condition  $E[k(X, X)] < \infty$ , there exists a unique covariance operator  $\mathbf{C}$  on  $\mathcal{H}$  such that

$$\text{Cov}[f(X), g(X)] = \langle f, \mathbf{C}g \rangle_k, \quad \forall f, g \in \mathcal{H}.$$

Moreover,  $\mathbf{C}$  induces the covariance operators  $\mathbf{C}_{00}$  and  $\mathbf{C}_{11}$  on  $\mathcal{H}^0$  and  $\mathcal{H}^1$ , and the cross-covariance operator  $\mathbf{C}_{01} : \mathcal{H}^1 \rightarrow \mathcal{H}^0$ . Also,  $\mathbf{C}_{01}$  has the representation

$$\mathbf{C}_{01} = \mathbf{C}_{00}^{1/2} \mathbf{V}_{01} \mathbf{C}_{11}^{1/2},$$

where  $\mathbf{V}_{01} : \mathcal{H}^1 \rightarrow \mathcal{H}^0$  is a unique bounded operator with  $\|\mathbf{V}_{01}\| \leq 1$ .

**Lemma 10.** *Let  $\mathcal{H} = \mathcal{H}^0 \oplus \mathcal{H}^1$  be a reproducing kernel Hilbert space with reproducing kernel  $k = k^0 + k^1$ , such that  $E[k(X, X)] < \infty$ , and let  $0 < a < b$  be absolute constants. Suppose  $\mathcal{H}^0$  is finite-dimensional with  $\mathbf{C}_{00} \succeq b\mathbf{I}$  and  $\|\mathbf{V}_{01}\| \leq \sqrt{1 - a/b}$ . Then for any  $\epsilon \in (0, a)$ ,*

$$\mathbf{C} - \epsilon \mathbf{P}^0 \succeq \mathbf{0}, \quad \mathbf{C} + \epsilon \mathbf{P}^1 \succeq \epsilon \mathbf{I}.$$

*Proof.* For any  $f \in \mathcal{H}$ , there is a unique decomposition  $f = f^0 + f^1$ , where  $f^0 \in \mathcal{H}^0$  and  $f^1 \in \mathcal{H}^1$ . Thus, it is straightforward to verify that

$$\langle f, (\mathbf{C} - \epsilon \mathbf{P}^0)f \rangle_k = \langle f^0, (\mathbf{C}_{00} - \epsilon \mathbf{I})f^0 \rangle_{k^0} + \langle f^1, \mathbf{C}_{11}f^1 \rangle_{k^1} + 2\langle f^0, \mathbf{C}_{01}f^1 \rangle_{k^0}.$$

The desired claim is true if we can show that

$$|\langle f^0, \mathbf{C}_{01}f^1 \rangle_{k^0}| \leq \|(\mathbf{C}_{00} - \epsilon \mathbf{I})^{1/2}f^0\|_{k^0} \|\mathbf{C}_{11}^{1/2}f^1\|_{k^1}. \quad (42)$$

To this end, using the fact that  $\mathbf{C}_{01} = \mathbf{C}_{00}^{1/2} \mathbf{V}_{01} \mathbf{C}_{11}^{1/2}$ , we get

$$\begin{aligned} |\langle f^0, \mathbf{C}_{01}f^1 \rangle_{k^0}| &= |\langle f^0, \mathbf{C}_{00}^{1/2} \mathbf{V}_{01} \mathbf{C}_{11}^{1/2} f^1 \rangle_{k^0}| \\ &= |\langle (\mathbf{C}_{00} - \epsilon \mathbf{I})^{1/2} f^0, (\mathbf{C}_{00} - \epsilon \mathbf{I})^{-1/2} \mathbf{C}_{00}^{1/2} \mathbf{V}_{01} \mathbf{C}_{11}^{1/2} f^1 \rangle_{k^0}| \\ &\leq \|(\mathbf{C}_{00} - \epsilon \mathbf{I})^{1/2} f^0\|_{k^0} \|(\mathbf{C}_{00} - \epsilon \mathbf{I})^{-1/2} \mathbf{C}_{00}^{1/2} \mathbf{V}_{01} \mathbf{C}_{11}^{1/2} f^1\|_{k^0} \\ &\leq \|(\mathbf{C}_{00} - \epsilon \mathbf{I})^{1/2} f^0\|_{k^0} \|\mathbf{C}_{11}^{1/2} f^1\|_{k^1} \|(\mathbf{C}_{00} - \epsilon \mathbf{I})^{-1/2} \mathbf{C}_{00}^{1/2} \mathbf{V}_{01}\|. \end{aligned}$$

Therefore, to establish (42) we only need to show that

$$\|(\mathbf{C}_{00} - \epsilon \mathbf{I})^{-1/2} \mathbf{C}_{00}^{1/2} \mathbf{V}_{01}\| \leq 1.$$

To this end, let  $\dim(\mathcal{H}^0) = m$ , then we have  $\mathbf{C}_{00} = \sum_{i=1}^m \lambda_i \langle \psi_i, \cdot \rangle_{k^0} \psi_i$ , where  $\lambda_i \geq b$  and the  $\psi_i$ 's are of unit norm. Hence,

$$(\mathbf{C}_{00} - \epsilon \mathbf{I})^{-1/2} \mathbf{C}_{00}^{1/2} = \sum_{i=1}^m \left( \frac{\lambda_i}{\lambda_i - \epsilon} \right)^{1/2} \langle \psi_i, \cdot \rangle_{k^0} \psi_i = \sum_{i=1}^m \left( \frac{1}{1 - \epsilon/\lambda_i} \right)^{1/2} \langle \psi_i, \cdot \rangle_{k^0} \psi_i,$$

and so

$$\begin{aligned} \|(\mathbf{C}_{00} - \epsilon \mathbf{I})^{-1/2} \mathbf{C}_{00}^{1/2} \mathbf{V}_{01}\| &\leq \|(\mathbf{C}_{00} - \epsilon \mathbf{I})^{-1/2} \mathbf{C}_{00}^{1/2}\| \|\mathbf{V}_{01}\| \\ &\leq \max_{1 \leq i \leq m} \left( \frac{1}{1 - \epsilon/\lambda_i} \right)^{1/2} \|\mathbf{V}_{01}\| \\ &\leq \left( \frac{1}{1 - \epsilon/b} \right)^{1/2} \|\mathbf{V}_{01}\| \\ &\leq \left( \frac{1}{1 - a/b} \right)^{1/2} \|\mathbf{V}_{01}\| \\ &\leq 1. \end{aligned}$$

This completes the proof.  $\square$

**Remark 4.** The condition that  $\mathcal{H}^0$  is finite-dimensional seems unavoidable. Since  $\mathbf{C}_{00}$  has to be trace class as in the definition of covariance operator, the additional condition  $\mathbf{C}_{00} \succeq b\mathbf{I}$  only makes sense when  $\dim(\mathcal{H}^0) < \infty$ .

With  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}$  now well-defined, we are ready to derive more of its properties, which will be useful later on.

**Lemma 11.** *Suppose that Assumptions 1 and 3 hold. Then for  $\epsilon$  sufficiently small, the operators  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1}$  and  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}$  are self-adjoint and bounded above by  $\epsilon^{-1}$  and  $\epsilon^{-1/2}$ , respectively. In addition,*

$$\begin{aligned} \|\mathbf{C}_{jj}^{1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{1/2}\| &\leq \epsilon^{1/2}, \\ \|(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \mathbf{C}_{jj}^{1/2}\| &= \|\mathbf{C}_{jj}^{1/2} (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \leq 2, \\ \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ij} (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| &\leq 4. \end{aligned}$$

*Proof.* Since the adjoint of the inverse of an operator is equal to the inverse of the adjoint of the operator, and  $\mathbf{C}_{jj}$  and  $\mathbf{P}_j^1$  are self-adjoint, we get

$$[(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1}]^* = [(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^*]^{-1} = (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1}.$$

Now given a positive self-adjoint operator  $A$ , if  $B$  is the unique square root of  $A$ , i.e.  $B^2 = A$ , then  $(B^*)^2 = (B^*)(B^*) = (B^2)^* = A^* = A$ , so by uniqueness of the square root of a positive self-adjoint operator we have  $B = B^*$ . This implies that  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}$  is self-adjoint.

Under Assumptions 1 and 3, we have  $\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1 \succeq \epsilon \mathbf{I}$  for  $\epsilon$  sufficiently small, by Lemma 10. It follows immediately that  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1}$  and  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}$  are bounded above by  $\epsilon^{-1}$  and  $\epsilon^{-1/2}$ , respectively.

Applying the inequality

$$\|A^{1/2} - B^{1/2}\| \leq \frac{\|A - B\|}{\lambda_{\min}(A^{1/2}) + \lambda_{\min}(B^{1/2})}$$

from Lemma 5 to  $A = \mathbf{C}_{jj}$  and  $B = \mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1$ , we get

$$\|\mathbf{C}_{jj}^{1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{1/2}\| \leq \frac{\epsilon}{0 + \epsilon^{1/2}} = \epsilon^{1/2}.$$

It follows that

$$\begin{aligned} \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - \mathbf{I}\| &= \|[\mathbf{C}_{jj}^{1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{1/2}](\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &\leq \|\mathbf{C}_{jj}^{1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{1/2}\| \|(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &\leq \epsilon^{1/2} \cdot \epsilon^{-1/2} \\ &= 1. \end{aligned}$$

By triangle inequality, we have

$$\|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \leq 2.$$

Since  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \mathbf{C}_{jj}^{1/2}$  is the adjoint of  $\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}$ , we immediately get  $\|(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \mathbf{C}_{jj}^{1/2}\| = \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \leq 2$ . From  $\|\mathbf{V}\| \leq 1$ , we get

$$\begin{aligned} &\|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ij}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &= \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} \mathbf{V}_{ij} \mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &\leq \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2}\| \|\mathbf{V}_{ij}\| \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &\leq 4. \end{aligned}$$

□

**Lemma 12.** *Conditioned on the event*

$$E_n = \left\{ \hat{\mathbf{C}}_{ii}^{(n)} + \epsilon_n \mathbf{P}_i^1 \succeq \frac{\epsilon_n}{2} \mathbf{I}, \hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1 \succeq \frac{\epsilon_n}{2} \mathbf{I} \right\},$$

*we have*

$$\begin{aligned} \|(\hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1)^{-1/2}(\hat{\mathbf{C}}_{jj}^{(n)})^{1/2}\| &= \|(\hat{\mathbf{C}}_{jj}^{(n)})^{1/2}(\hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1)^{-1/2}\| \leq 3, \\ \|(\hat{\mathbf{C}}_{ii}^{(n)} + \epsilon_n \mathbf{P}_i^1)^{-1/2} \hat{\mathbf{C}}_{ij}^{(n)}(\hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1)^{-1/2}\| &\leq 9. \end{aligned}$$

*Proof.* The proof is essentially the same as that in Lemma 11 except that the event

$$\{\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1 \succeq \epsilon \mathbf{I} \text{ and } \mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1 \succeq \epsilon \mathbf{I}\}$$

is now replaced by  $E_n$ .

□

**Lemma 13.** Let  $\epsilon_n$  be a sequence of positive numbers such that

$$\lim_{n \rightarrow \infty} \epsilon_n = 0, \quad \lim_{n \rightarrow \infty} \frac{n^{-1/2}}{\epsilon_n} = 0.$$

Then, under Assumptions 1 and 3,

$$\begin{aligned} P\left(\hat{\mathbf{C}}_{ii}^{(n)} + \epsilon_n \mathbf{P}_i^1 \succeq \frac{\epsilon_n}{2} \mathbf{I}, \hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1 \succeq \frac{\epsilon_n}{2} \mathbf{I}\right) &\geq 1 - \delta, \\ P\left(\hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1 \succeq \frac{\epsilon_n}{2} \mathbf{I} \text{ for } 1 \leq j \leq p\right) &\geq 1 - \delta', \end{aligned}$$

where  $\delta = 2(d_i + d_j)\epsilon^{-1}n^{-1/2}$ ,  $\delta' = 2dp\epsilon^{-1}n^{-1/2}$ , and  $d_i, d_j, d$  are constants that do not depend on  $n$  when  $n$  is sufficiently large.

*Proof.* To simplify notation, we write  $\epsilon$  for  $\epsilon_n$  and  $\hat{\mathbf{C}}_{jj}$  for  $\hat{\mathbf{C}}_{jj}^{(n)}$ . Then by Lemma 9,

$$\begin{aligned} P(\|\hat{\mathbf{C}}_{jj} - \mathbf{C}_{jj}\| > \epsilon) &\leq P(\|\hat{\mathbf{C}}_{jj} - \mathbf{C}_{jj}\|_{\text{HS}} > \epsilon) \\ &\leq \epsilon^{-1} E\|\hat{\mathbf{C}}_{jj} - \mathbf{C}_{jj}\|_{\text{HS}} \\ &\leq d_j \epsilon^{-1} n^{-1/2}, \end{aligned} \tag{43}$$

where  $d_j$  is some constant that does not depend on  $n$  when  $n$  is sufficiently large.

By Lemma 10, under Assumptions 1 and 3, we have  $\mathbf{C}_{jj} - \epsilon \mathbf{P}_j^0 \succeq \mathbf{0}$ , so

$$\begin{aligned} \hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1 &= \left[ \hat{\mathbf{C}}_{jj} - \epsilon \mathbf{P}_j^0 + \frac{\epsilon}{2} \mathbf{I} \right] + \frac{\epsilon}{2} \mathbf{I} \\ &= \left[ \hat{\mathbf{C}}_{jj} - \mathbf{C}_{jj} + \frac{\epsilon}{2} \mathbf{I} \right] + \left[ \mathbf{C}_{jj} - \epsilon \mathbf{P}_j^0 \right] + \frac{\epsilon}{2} \mathbf{I} \\ &\succeq \left[ \hat{\mathbf{C}}_{jj} - \mathbf{C}_{jj} + \frac{\epsilon}{2} \mathbf{I} \right] + \frac{\epsilon}{2} \mathbf{I}. \end{aligned}$$

It follows that

$$\begin{aligned} P\left(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1 \succeq \frac{\epsilon}{2} \mathbf{I}\right) &\geq P\left(\hat{\mathbf{C}}_{jj} - \mathbf{C}_{jj} + \frac{\epsilon}{2} \mathbf{I} \succeq \mathbf{0}\right) \\ &= P\left(\mathbf{C}_{jj} - \hat{\mathbf{C}}_{jj} \preceq \frac{\epsilon}{2} \mathbf{I}\right) \\ &\geq P\left(\|\mathbf{C}_{jj} - \hat{\mathbf{C}}_{jj}\| \leq \frac{\epsilon}{2}\right) \\ &\geq 1 - 2d_j \epsilon^{-1} n^{-1/2}, \end{aligned}$$

the last inequality is due to (43). Hence

$$\begin{aligned} &P\left(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1 \succeq \frac{\epsilon}{2} \mathbf{I}, \hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1 \succeq \frac{\epsilon}{2} \mathbf{I}\right) \\ &= 1 - P\left(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1 \preceq \frac{\epsilon}{2} \mathbf{I} \text{ or } \hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1 \preceq \frac{\epsilon}{2} \mathbf{I}\right) \\ &\geq 1 - P\left(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1 \preceq \frac{\epsilon}{2} \mathbf{I}\right) - P\left(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1 \preceq \frac{\epsilon}{2} \mathbf{I}\right) \\ &\geq 1 - \delta, \end{aligned}$$

where  $\delta = 2(d_i + d_j)\epsilon^{-1}n^{-1/2}$ . Let  $d = \max\{d_1, \dots, d_p\}$  and apply union bound yields  $\delta' = 2dp\epsilon^{-1}n^{-1/2}$ .  $\square$

**Lemma 14.** Suppose that Assumptions 1 and 3 hold. Let  $f$  be an eigenfunction of  $\mathbf{C}_{ii}$  corresponding to a nonzero eigenvalue  $\lambda$ , with the unique decomposition  $f = f^0 + f^1$ , where  $f^0 \in \mathcal{H}_i^0$  and  $f^1 \in \mathcal{H}_i^1$ . Then, for  $\epsilon$  sufficiently small,

$$(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} f = \lambda^{-1} (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f - \lambda^{-1} \epsilon (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} f^1. \quad (44)$$

*Proof.* We have

$$(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1) f = \lambda f + \epsilon f^1.$$

Applying  $(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1}$  on both sides and rearranging terms, we get

$$(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1} f = \lambda^{-1} f - \lambda^{-1} \epsilon (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1} f^1.$$

Applying  $(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2}$  on both sides, we get

$$(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} f = \lambda^{-1} (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f - \lambda^{-1} \epsilon (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} f^1.$$

$\square$

### A.3 Proofs of Main Lemmas

We are now ready to prove the two key lemmas given in Section 6.

#### Proof of Lemma 3

*Proof.* Throughout, we condition on the event

$$E_n = \left\{ \hat{\mathbf{C}}_{ii}^{(n)} + \epsilon_n \mathbf{P}_i^1 \succeq \frac{\epsilon_n}{2} \mathbf{I}, \hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1 \succeq \frac{\epsilon_n}{2} \mathbf{I} \right\}. \quad (45)$$

It follows from Lemma 13 that  $P(E_n) \geq 1 - \delta$  with  $\delta = 2(d_i + d_j)\epsilon_n^{-1}n^{-1/2}$ , and  $d_i, d_j$  are constants that do not depend on  $n$  when  $n$  is sufficiently large.

To simplify notation, we write  $\epsilon$  for  $\epsilon_n$  and  $\hat{\mathbf{C}}_{ij}$  for  $\hat{\mathbf{C}}_{ij}^{(n)}$  hereinafter. First, note that the operator on the left hand side of (27) can be decomposed as

$$\begin{aligned} & \hat{\mathbf{V}}_{ij}^{(n)} - \tilde{\mathbf{V}}_{ij}^{(n)} \\ &= (\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \hat{\mathbf{C}}_{ij} (\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \\ & \quad - (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ij} (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \\ &= \{(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} - (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2}\} \hat{\mathbf{C}}_{ij} (\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \\ & \quad + (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \{\hat{\mathbf{C}}_{ij} - \mathbf{C}_{ij}\} (\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \\ & \quad + (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ij} \{(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\}. \end{aligned} \quad (46)$$

$$+ (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \{\hat{\mathbf{C}}_{ij} - \mathbf{C}_{ij}\} (\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \quad (47)$$

$$+ (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ij} \{(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\}. \quad (48)$$

We now bound each term on the right hand side of the equation above separately. From the equality

$$\begin{aligned} A^{-1/2} - B^{-1/2} &= A^{-1/2} (B^{3/2} - A^{3/2}) B^{-3/2} + (A - B) B^{-3/2} \\ &= [A^{-1/2} (B^{3/2} - A^{3/2}) + A - B] B^{-3/2}, \end{aligned}$$

plug in  $A = \mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1$ ,  $B = \hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1$ , and (46) becomes

$$\begin{aligned} & -(A^{-1/2} - B^{-1/2})\hat{\mathbf{C}}_{ij}(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \\ &= -[A^{-1/2}(B^{3/2} - A^{3/2}) + A - B]B^{-3/2}\hat{\mathbf{C}}_{ij}(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \\ &= -[A^{-1/2}(B^{3/2} - A^{3/2}) + A - B] \cdot (\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{-3/2}\hat{\mathbf{C}}_{ij}(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}. \end{aligned} \quad (49)$$

Now, we bound each term in the product in (49). Under Assumptions 1 and 3, by Lemma 11, we have  $\|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2}\| \leq \epsilon^{-1/2}$ , so

$$\begin{aligned} & \|A^{-1/2}(B^{3/2} - A^{3/2}) + A - B\| \\ &= \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2}\{(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{3/2} - (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{3/2}\} + \mathbf{C}_{ii} - \hat{\mathbf{C}}_{ii}\| \\ &\leq \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2}\| \cdot \|(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{3/2} - (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{3/2}\| + \|\mathbf{C}_{ii} - \hat{\mathbf{C}}_{ii}\| \\ &\leq \epsilon^{-1/2} \cdot 3\lambda^{1/2}\|\mathbf{C}_{ii} - \hat{\mathbf{C}}_{ii}\| + \|\mathbf{C}_{ii} - \hat{\mathbf{C}}_{ii}\| \\ &\quad \text{where } \lambda = \max\{\|\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1\|, \|\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1\|\}, \text{ by Lemma 6} \\ &= \left(3\lambda^{1/2}\epsilon^{-1/2} + 1\right)\|\mathbf{C}_{ii} - \hat{\mathbf{C}}_{ii}\| \\ &= O(\epsilon^{-1/2}n^{-1/2}), \quad \text{by Lemma 9.} \end{aligned} \quad (50)$$

To bound the other term in (49), it follows from Lemma 12 that conditioned on (45), we have  $\|(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{-1}\| \leq 2\epsilon^{-1}$  and  $\|(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2}\hat{\mathbf{C}}_{ij}(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \leq 9$ . Therefore,

$$\begin{aligned} & \|(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{-3/2}\hat{\mathbf{C}}_{ij}(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &= \|(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{-1}\| \|(\hat{\mathbf{C}}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2}\hat{\mathbf{C}}_{ij}(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &\leq 18\epsilon^{-1}, \end{aligned} \quad (51)$$

Combining (50) and (51), we see that the norm of (46) is of order  $O(\epsilon^{-3/2}n^{-1/2})$ . A similar bound can be obtained for (48). An upper bound for (47) is given by  $2\epsilon^{-1}\|\mathbf{C}_{ij} - \hat{\mathbf{C}}_{ij}\| = O(\epsilon^{-1}n^{-1/2})$ .  $\square$

We now turn to the proof of Lemma 4.

### Proof of Lemma 4

*Proof.* To simplify notation, we write  $\epsilon$  for  $\epsilon_n$ . First, we rewrite the left hand side of (28) as

$$\begin{aligned} \|\tilde{\mathbf{V}}_{ij}^{(n)} - \mathbf{V}_{ij}\| &= \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2}\mathbf{C}_{ij}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - \mathbf{C}_{ii}^{-1/2}\mathbf{C}_{ij}\mathbf{C}_{jj}^{-1/2}\| \\ &\leq \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} - \mathbf{C}_{ii}^{-1/2}\|\mathbf{C}_{ij}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &\quad + \|\mathbf{C}_{ii}^{-1/2}\mathbf{C}_{ij}\{(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - \mathbf{C}_{jj}^{-1/2}\}\|. \end{aligned} \quad (52)$$

$$\quad \quad \quad (53)$$

Applying Lemma 11, an upper bound for (52) is given by

$$\begin{aligned} & \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} - \mathbf{C}_{ii}^{-1/2}\|\mathbf{C}_{ij}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &= \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} - \mathbf{C}_{ii}^{-1/2}\|\mathbf{C}_{ii}^{1/2}\mathbf{V}_{ij}\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \\ &\leq 2\|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} - \mathbf{C}_{ii}^{-1/2}\|\mathbf{C}_{ii}^{1/2}\mathbf{V}_{ij}\| \\ &= 2\|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2}\mathbf{C}_{ii}^{1/2} - \mathbf{I}\|\mathbf{V}_{ij}\|. \end{aligned}$$

Our goal is to show that

$$\|\{(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} - \mathbf{I}\} \mathbf{V}_{ij}\| \longrightarrow 0 \text{ as } n \longrightarrow \infty. \quad (54)$$

Let  $f$  be a unit eigenfunction of  $\mathbf{C}_{ii}$  corresponding to a nonzero eigenvalue  $\lambda$ . It follows from Lemma 14 that

$$\begin{aligned} & \|\{(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} - \mathbf{I}\} \mathbf{C}_{ii} f\|_{k_i} \\ &= \lambda \|\{(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} - \mathbf{I}\} f\|_{k_i} \\ &= \lambda \left\| \lambda^{1/2} \left\{ \lambda^{-1} (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f - \lambda^{-1} \epsilon (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} f^1 \right\} - f \right\|_{k_i} \\ &\leq \lambda \left[ \|\lambda^{-1/2} (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f - f\|_{k_i} + \epsilon \lambda^{-1/2} \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} f^1\|_{k_i} \right] \\ &= \lambda \|\lambda^{-1/2} (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f - f\|_{k_i} + \epsilon \lambda^{1/2} \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} f^1\|_{k_i}. \end{aligned} \quad (55)$$

To bound the first term in (55), note that from Lemma 11,

$$\begin{aligned} |\langle f, (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f \rangle_{k_i} - \langle f, \mathbf{C}_{ii}^{1/2} f \rangle_{k_i}| &= |\langle f, [(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} - \mathbf{C}_{ii}^{1/2}] f \rangle_{k_i}| \\ &\leq \|(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} - \mathbf{C}_{ii}^{1/2}\| \\ &\leq \epsilon^{1/2}, \end{aligned}$$

so we have

$$\begin{aligned} & \|\lambda^{-1/2} (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f - f\|_{k_i}^2 \\ &= \lambda^{-1} \langle f, (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1) f \rangle_{k_i} - 2\lambda^{-1/2} \langle f, (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f \rangle_{k_i} + \|f\|_{k_i}^2 \\ &\leq \lambda^{-1} (\lambda + \epsilon \|f^1\|^2) - 2\lambda^{-1/2} [\langle f, \mathbf{C}_{ii}^{1/2} f \rangle_{k_i} - \epsilon^{1/2}] + 1 \\ &= 2 + \lambda^{-1} \epsilon \|f^1\|^2 - 2\lambda^{-1/2} \cdot \lambda^{1/2} + 2\lambda^{-1/2} \epsilon^{1/2} \\ &\leq \lambda^{-1} \epsilon + 2\lambda^{-1/2} \epsilon^{1/2}, \end{aligned}$$

which gives

$$\begin{aligned} \|\lambda^{-1/2} (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{1/2} f - f\|_{k_i} &\leq [\lambda^{-1} \epsilon + 2\lambda^{-1/2} \epsilon^{1/2}]^{1/2} \\ &\leq \lambda^{-1/2} \epsilon^{1/2} + \sqrt{2} \lambda^{-1/4} \epsilon^{1/4} \\ &\leq \lambda^{-1/2} \epsilon^{1/2} + 2\lambda^{-1/4} \epsilon^{1/4}. \end{aligned}$$

It follows that an upper bound for the expression on the left hand side of (55) is

$$\begin{aligned} \|\{(\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} - \mathbf{I}\} \mathbf{C}_{ii} f\|_{k_i} &\leq \lambda \cdot (\lambda^{-1/2} \epsilon^{1/2} + 2\lambda^{-1/4} \epsilon^{1/4}) + \epsilon \lambda^{1/2} \cdot \epsilon^{-1/2} \\ &= 2(\lambda \epsilon)^{1/2} + 2\lambda^{3/4} \epsilon^{1/4}. \end{aligned} \quad (56)$$

As pointed out in Section 6.2,  $\mathcal{R}(\mathbf{V}_{ij}) \subseteq \overline{\mathcal{R}(\mathbf{C}_{ii})}$ . Now, let  $v$  be an arbitrary element in  $\mathcal{R}(\mathbf{V}_{ij}) \cap \mathcal{R}(\mathbf{C}_{ii})$ , so that there exists  $u \in \mathcal{H}_i$  such that  $v = \mathbf{C}_{ii} u$ . We then have  $u = \sum_{\ell=1}^{\infty} \langle u, f_{\ell} \rangle_{k_i} f_{\ell}$ , where  $f_{\ell}$  is a unit eigenvector of  $\mathbf{C}_{ii}$  corresponding to nonzero eigenvalue  $\lambda_{\ell}$  (i.e.,  $\{f_{\ell}\}$  and the eigenfunctions

corresponding to zero eigenvalue forms an orthonormal basis system of  $\mathcal{H}_i$ ), and

$$\begin{aligned}
& \| \{ (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} - \mathbf{I} \} v \|_{k_i} \\
&= \| \{ (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} - \mathbf{I} \} \mathbf{C}_{ii} u \|_{k_i} \\
&\leq \sum_{\ell=1}^{\infty} | \langle u, f_{\ell} \rangle_{k_i} | \| \{ (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} - \mathbf{I} \} \mathbf{C}_{ii} f_{\ell} \|_{k_i} \\
&\leq \sum_{\ell=1}^{\infty} | \langle u, f_{\ell} \rangle_{k_i} | \cdot [2(\lambda_{\ell} \epsilon)^{1/2} + 2\lambda_{\ell}^{3/4} \epsilon^{1/4}] \\
&\leq \left( \sum_{\ell=1}^{\infty} \langle u, f_{\ell} \rangle_{k_i}^2 \right)^{1/2} \left( \sum_{\ell=1}^{\infty} 4\lambda_{\ell} \epsilon \right)^{1/2} \\
&\quad + 2\epsilon^{1/4} \left\{ \sum_{\ell: \lambda_{\ell} \geq 1} | \langle u, f_{\ell} \rangle_{k_i} | \lambda_{\ell} + \sum_{\ell: 0 < \lambda_{\ell} < 1} | \langle u, f_{\ell} \rangle_{k_i} | \lambda_{\ell}^{1/2} \right\} \\
&\leq 2\epsilon^{1/2} \|u\|_{k_i} \left( \sum_{\ell=1}^{\infty} \lambda_{\ell} \right)^{1/2} + 2\epsilon^{1/4} \left\{ \|u\|_{k_i} \sum_{\ell: \lambda_{\ell} \geq 1} \lambda_{\ell} + \|u\|_{k_i} \left( \sum_{\ell: 0 < \lambda_{\ell} < 1} \lambda_{\ell} \right)^{1/2} \right\} \\
&= O(\epsilon^{1/4}),
\end{aligned}$$

where the second inequality follows from (56), the third and fourth inequality follows from Cauchy-Schwarz inequality, and the last equality follows from the fact that  $\mathbf{C}_{ii}$  is trace class and hence  $\sum_{\ell=1}^{\infty} \lambda_{\ell} < \infty$ . We therefore conclude that

$$\{ (\mathbf{C}_{ii} + \epsilon \mathbf{P}_i^1)^{-1/2} \mathbf{C}_{ii}^{1/2} - \mathbf{I} \} v \longrightarrow 0 \text{ for all } v \in \mathcal{R}(\mathbf{V}_{ij}) \cap \mathcal{R}(\mathbf{C}_{ii}) \text{ as } n \longrightarrow \infty. \quad (57)$$

Coupled with that fact that  $\mathbf{V}_{ij}$  is compact, Lemma 7 implies that (54) holds.

To show the convergence of (53), first note that we can rewrite (53) as

$$\begin{aligned}
\| \mathbf{C}_{ii}^{-1/2} \mathbf{C}_{ij} \{ (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - \mathbf{C}_{jj}^{-1/2} \} \| &= \| \mathbf{V}_{ij} \mathbf{C}_{jj}^{1/2} \{ (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - \mathbf{C}_{jj}^{-1/2} \} \| \\
&= \| \mathbf{V}_{ij} \{ \mathbf{C}_{jj}^{1/2} (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - \mathbf{I} \} \|.
\end{aligned}$$

Using the fact that  $(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}$  is self-adjoint, we get

$$\begin{aligned}
\| \mathbf{V}_{ij} \{ \mathbf{C}_{jj}^{1/2} (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - \mathbf{I} \} \| &= \| (\mathbf{V}_{ij} \{ \mathbf{C}_{jj}^{1/2} (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - \mathbf{I} \})^* \| \\
&= \| \{ (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \mathbf{C}_{jj}^{1/2} - \mathbf{I} \} \mathbf{V}_{ij}^* \|.
\end{aligned}$$

Since  $\mathbf{V}_{ij}$  is compact implies that  $\mathbf{V}_{ij}^*$  is compact, it follows similarly from our proof for (57) and an application of Lemma 7 that

$$\| \{ (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \mathbf{C}_{jj}^{1/2} - \mathbf{I} \} \mathbf{V}_{ij}^* \| \longrightarrow 0.$$

□

## A.4 Proofs of Main Theorems

### Proof of Theorem 2

*Proof.* It follows from Lemmas 3 and 4 that we have

$$\| \hat{\mathbf{V}}_{ij}^{(n)} - \mathbf{V}_{ij} \| \longrightarrow 0$$



in probability when  $n \rightarrow \infty$ . From the expression in (25), we see that

$$\mathbf{V} = \sum_{i=1}^p \sum_{j \neq i} \mathbf{P}_i \mathbf{V} \mathbf{P}_j + \mathbf{I},$$

where  $\mathbf{P}_j$  is the orthogonal projection from  $\mathcal{H}$  onto  $\mathcal{H}_j$  and  $\mathbf{I} : \mathcal{H} \rightarrow \mathcal{H}$  is the identity operator. Since there is a one-to-one correspondence between  $\mathbf{V}_{ij}$  and  $\mathbf{P}_i \mathbf{V} \mathbf{P}_j$  (for  $i \neq j$ ), using a similar decomposition for  $\hat{\mathbf{V}}^{(n)}$ , we get

$$\|\hat{\mathbf{V}}^{(n)} - \mathbf{V}\| \leq \sum_{i=1}^p \sum_{j \neq i} \|\hat{\mathbf{V}}_{ij}^{(n)} - \mathbf{V}_{ij}\| \rightarrow 0$$

in probability as  $n \rightarrow \infty$ . It then follows from Lemma 8 that

$$|\langle \hat{\mathbf{f}}^{(n)}, \mathbf{f}^* \rangle_k| \rightarrow 1$$

in probability as  $n \rightarrow \infty$ . □

### Proof of Theorem 1

*Proof.* Throughout, we condition on the event

$$F_n = \left\{ \hat{\mathbf{C}}_{jj}^{(n)} + \epsilon_n \mathbf{P}_j^1 \succeq \frac{\epsilon_n}{2} \mathbf{I} \quad \text{for } 1 \leq j \leq p \right\}, \quad (58)$$

where  $P(F_n) \geq 1 - \delta$  with  $\delta = 2dp\epsilon_n^{-1}n^{-1/2}$  from Lemma 13, and  $d$  is a constant that does not depend on  $n$  when  $n$  is sufficiently large.

To simplify notation, we write  $\epsilon$  for  $\epsilon_n$  and  $\hat{\mathbf{C}}_{ij}$  for  $\hat{\mathbf{C}}_{ij}^{(n)}$ . Since

$$\sum_{j=1}^p \text{Var} [\hat{\phi}_j^{(n)} - \phi_j^*] = \sum_{j=1}^p \langle \hat{\phi}_j^{(n)} - \phi_j^*, \mathbf{C}_{jj}(\hat{\phi}_j^{(n)} - \phi_j^*) \rangle_{k_j} = \sum_{j=1}^p \|\mathbf{C}_{jj}^{1/2}(\hat{\phi}_j^{(n)} - \phi_j^*)\|_{k_j}^2,$$

it suffices to show that  $\|\mathbf{C}_{jj}^{1/2}(\hat{\phi}_j^{(n)} - \phi_j^*)\|_{k_j} \rightarrow 0$  in probability as  $n \rightarrow \infty$ . Using the fact that  $\hat{f}_j^{(n)} = (\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{1/2} \hat{\phi}_j^{(n)}$ ,  $f_j^* = \mathbf{C}_{jj}^{1/2} \phi_j^*$ , we have

$$\begin{aligned} \|\mathbf{C}_{jj}^{1/2}(\hat{\phi}_j^{(n)} - \phi_j^*)\|_{k_j} &= \|\mathbf{C}_{jj}^{1/2}(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} \hat{f}_j^{(n)} - f_j^*\|_{k_j} \\ &\leq \|\mathbf{C}_{jj}^{1/2}\{(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\} \hat{f}_j^{(n)}\|_{k_j} \end{aligned} \quad (59)$$

$$+ \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}(\hat{f}_j^{(n)} - f_j^*)\|_{k_j} \quad (60)$$

$$+ \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} f_j^* - f_j^*\|_{k_j}. \quad (61)$$

An upper bound for (59) can be obtained using similar argument as that in the bound for (46). First, consider the equality

$$\begin{aligned} A^{-1/2} - B^{-1/2} &= A^{-3/2}(B^{3/2} - A^{3/2})B^{-1/2} + A^{-3/2}(A - B) \\ &= A^{-3/2}[(B^{3/2} - A^{3/2})B^{-1/2} + A - B], \end{aligned}$$

and plug in  $A = \mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1$  and  $B = \hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1$ , in which case the operator in (59) becomes

$$\begin{aligned}
& -\mathbf{C}_{jj}^{1/2}(A^{-1/2} - B^{-1/2}) \\
& = -\mathbf{C}_{jj}^{1/2}A^{-3/2}[(B^{3/2} - A^{3/2})B^{-1/2} + A - B] \\
& = -\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-3/2}[(B^{3/2} - A^{3/2})B^{-1/2} + A - B]
\end{aligned} \tag{62}$$

Now we bound each term in the product (62). Since

$$\begin{aligned}
\|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-3/2}\| & \leq \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \|(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1}\| \\
& \leq 2\epsilon^{-1},
\end{aligned} \tag{63}$$

and

$$\begin{aligned}
& \|(B^{3/2} - A^{3/2})B^{-1/2} + A - B\| \\
& = \|\{(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{3/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{3/2}\}(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2} + \mathbf{C}_{jj} - \hat{\mathbf{C}}_{jj}\| \\
& \leq \|(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{3/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{3/2}\| \|(\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| + \|\mathbf{C}_{jj} - \hat{\mathbf{C}}_{jj}\| \\
& \leq 3\lambda^{1/2}\|\hat{\mathbf{C}}_{jj} - \mathbf{C}_{jj}\| \cdot \sqrt{2}\epsilon^{-1/2} + \|\mathbf{C}_{jj} - \hat{\mathbf{C}}_{jj}\| \\
& \quad \text{where } \lambda = \max\{\|\hat{\mathbf{C}}_{jj} + \epsilon \mathbf{P}_j^1\|, \|\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1\|\}, \text{ by Lemma 6} \\
& = \left(3\sqrt{2}\lambda^{1/2}\epsilon^{-1/2} + 1\right)\|\mathbf{C}_{jj} - \hat{\mathbf{C}}_{jj}\| \\
& = O(\epsilon^{-1/2}n^{-1/2}),
\end{aligned} \tag{64}$$

combining (63) and (64) gives an upper bound of order  $O(\epsilon^{-3/2}n^{-1/2})$  on (59).

For (60), it follows from Theorem 2 that

$$\begin{aligned}
\|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}(\hat{f}_j^{(n)} - f_j^*)\|_{k_j} & \leq \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \|\hat{f}_j^{(n)} - f_j^*\|_{k_j} \\
& \leq 2\|\hat{f}_j^{(n)} - f_j^*\|_{k_j} \longrightarrow 0
\end{aligned}$$

in probability as  $n \longrightarrow \infty$ . Finally, for (61), using the fact that  $f_j^* = \mathbf{C}_{jj}^{1/2}\phi_j^*$ , we get

$$\begin{aligned}
& \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}f_j^* - f_j^*\|_{k_j} \\
& = \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\mathbf{C}_{jj}^{1/2}\phi_j^* - \mathbf{C}_{jj}^{1/2}\phi_j^*\|_{k_j} \\
& = \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\{\mathbf{C}_{jj}^{1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{1/2}\}\phi_j^*\|_{k_j} \\
& \leq \|\mathbf{C}_{jj}^{1/2}(\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{-1/2}\| \|\mathbf{C}_{jj}^{1/2} - (\mathbf{C}_{jj} + \epsilon \mathbf{P}_j^1)^{1/2}\| \|\phi_j^*\|_{k_j} \\
& \leq 2\|\phi_j^*\|_{k_j}\epsilon^{1/2} \longrightarrow 0,
\end{aligned}$$

the second inequality follows from Lemma 11. □

## B Supporting Proofs for Theorems in Section 7

This section contains proofs for theorems in Section 7. We present some facts about RKHS in Section B.1, followed by proofs of theorems in Section B.2.

### B.1 Properties of Reproducing Kernel Hilbert Spaces

The following properties of RKHS's will be useful for proving theorems in Section 7.

**Lemma 15.** *Let  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  be a kernel and  $\mathcal{H}$  its associated reproducing kernel Hilbert space. Then  $\mathcal{H} \subset C(\mathcal{X})$  if and only if  $\sup_{x \in \mathcal{X}} k(x, x) < \infty$  and  $k(x, \cdot)$  is continuous on  $\mathcal{X}$  for all  $x \in \mathcal{X}$ . Moreover, the inclusion  $\mathcal{H} \hookrightarrow C(\mathcal{X})$  is continuous.*

*Proof.* If  $\mathcal{H} \subset C(\mathcal{X})$ , then  $k(x, \cdot) \in C(\mathcal{X})$ . Moreover, for each  $f \in \mathcal{H}$ , we have  $|\langle k_x, f \rangle_k| = |f(x)| \leq \|f\|_\infty$  for all  $x \in \mathcal{X}$ . The principle of uniform boundedness implies that there exists  $M < \infty$  such that  $\|k_x\|_k \leq M$  for all  $x \in \mathcal{X}$ . It follows that  $\sup_{x \in \mathcal{X}} k(x, x) \leq M^2 < \infty$ .

Conversely, assume that  $k(x, x) \leq M^2$  and  $k(x, \cdot) \in C(\mathcal{X})$  for all  $x \in \mathcal{X}$ . Given  $f \in \mathcal{H}$ , we have

$$|f(x)| = |\langle f, k_x \rangle_k| \leq \|f\|_k \|k_x\|_k = \|f\|_k \sqrt{k(x, x)} \leq M \|f\|_k, \quad \forall x \in \mathcal{X}. \quad (65)$$

Hence, convergence in  $\mathcal{H}$  implies uniform convergence, so the closure of  $\text{span}\{k(x, \cdot) : x \in \mathcal{X}\}$  (with respect to  $\|\cdot\|_k$ ) is contained in  $C(\mathcal{X})$ , i.e.  $\mathcal{H} \subset C(\mathcal{X})$ . The continuity of inclusion follows from  $\|f\|_\infty \leq M \|f\|_k$ .  $\square$

**Corollary 2.** *Let  $\{f_n\} \subset \mathcal{H}$ , then  $\|f_n - f\|_k \rightarrow 0$  for some  $f \in \mathcal{H}$  implies that  $\|f_n - f\|_\infty \rightarrow 0$ .*

*Proof.* Immediate from (65).  $\square$

**Lemma 16.** *Let  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  be a kernel and  $\mathcal{H}$  its associated reproducing kernel Hilbert space. Let  $X$  be a random variable taking values in  $\mathcal{X}$  with induced probability measure  $P$  on  $\mathcal{X}$ . Then  $E[k(X, X)] < \infty$  implies that  $\mathcal{H} \subset L^2(\mathcal{X}, dP)$ , and the inclusion  $\mathcal{H} \hookrightarrow L^2(\mathcal{X}, dP)$  is continuous.*

*Proof.* The claim follows from

$$E[f^2(X)] = E[\langle f, k(X, \cdot) \rangle_k^2] \leq E[\|f\|_k^2 \|k(X, \cdot)\|_k^2] = \|f\|_k^2 E[k(X, X)], \quad \forall f \in \mathcal{H}.$$

$\square$

The readers are referred to [Reed and Simon \(1980\)](#), [Schölkopf and Smola \(2002\)](#) and [Aronszajn \(1950\)](#) for more details on functional analysis, kernel methods and reproducing kernels, respectively.

### B.2 Proofs

When Assumption 1 holds and  $\mathcal{H}_j^0$  excludes constants, for  $f \in \mathcal{H}_j^0$ ,  $\|f\|_{p_j}^2 := \text{Var}[f(X_j)] = 0$  if and only if  $f \equiv 0$ . By Remark 2, this implies that  $\mathcal{H}_j^0$  can be turned into an RKHS with inner product  $\langle \cdot, \cdot \rangle_{P_j}$ . Without loss of generality, in the following proofs, we define  $\langle \cdot, \cdot \rangle_{k_j^0} := \langle \cdot, \cdot \rangle_{P_j}$ .

### Proof of Theorem 3

*Proof.* To simplify notation, we omit the subscript  $j$ . Also, we define the semi-norm

$$\langle f, g \rangle_P := \text{Cov}[f(X), g(X)], \quad f, g \in L^2(\mathcal{X}, dP),$$

where  $X$  is a random variable taking values in  $\mathcal{X}$  with probability distribution  $P$ .

We first check that  $\langle \cdot, \cdot \rangle_*$  defines an appropriate inner product on  $\mathcal{H}$ . Clearly,  $\langle \cdot, \cdot \rangle_*$  is symmetric, bilinear and positive semi-definite. When  $f = f^0 + f^1$  with  $f^0 \in \mathcal{H}^0, f^1 \in \mathcal{H}^1$  satisfies  $\|f\|_* = 0$ , we have  $\|f^1\|_{k^1} = 0$  and  $\text{Var}[f(X)] = 0$ . This in turn implies that  $f^1 \equiv 0$ , and  $f^0$  is a constant function almost surely. Since  $\mathcal{H}^0 \subset C(\mathcal{X})$  and  $\mathcal{H}^0$  excludes constant, this means that  $f^0 \equiv 0$ . Therefore,  $f \equiv 0$  if and only if  $\|f\|_* = 0$ .

To see that  $\mathcal{H}$  is a Hilbert space with respect to  $\langle \cdot, \cdot \rangle_*$ , we need to show that if  $\{f_n\}$  is a Cauchy sequence in  $\mathcal{H}$  with respect to  $\|\cdot\|_*$ , then  $\{f_n\}$  converges in the norm  $\|\cdot\|_*$  to some  $f^* \in \mathcal{H}$ . So suppose that  $\{f_n\}$  is Cauchy with respect to  $\|\cdot\|_*$ , then it is also Cauchy with respect to  $\|\cdot\|_{k^1}$  and  $\|\cdot\|_P$ . We decompose  $f_n = f_n^0 + f_n^1$ , with  $f_n^0 \in \mathcal{H}^0$  and  $f_n^1 \in \mathcal{H}^1$ . Since  $\|f_n\|_{k^1} = \|f_n^1\|_{k^1}$ , and  $\mathcal{H}^1$  is itself an RKHS with respect to  $\langle \cdot, \cdot \rangle_{k^1}$ , we see that  $\{f_n^1\}$  is a Cauchy sequence in  $\mathcal{H}^1$ , so there exists a unique  $f^{*1} \in \mathcal{H}^1$  such that

$$\|f_n^1 - f^{*1}\|_{k^1} \longrightarrow 0. \quad (66)$$

On the other hand, by Corollary 2 we know that  $\|f_n^1 - f^{*1}\|_{k^1} \longrightarrow 0$  implies  $\|f_n^1 - f^{*1}\|_\infty \longrightarrow 0$ . So

$$\|f_n^1 - f^{*1}\|_P \leq 2\|f_n^1 - f^{*1}\|_\infty \longrightarrow 0. \quad (67)$$

Now we consider  $\{f_n^0\}$ , and we want to show that there exists  $f^{*0} \in \mathcal{H}^0$  such that  $\|f_n^0 - f^{*0}\|_P \longrightarrow 0$ . We know that  $\{f_n\}$  and  $\{f_n^1\}$  are Cauchy with respect to  $\|\cdot\|_P$ , so for every  $\epsilon > 0$ , there exists  $N(\epsilon)$  such that if  $m \geq n \geq N(\epsilon)$ , we have

$$\|f_n^0 - f_m^0 + f_n^1 - f_m^1\|_P = \|f_n - f_m\|_P < \frac{\epsilon}{2}, \quad \text{and} \quad \|f_n^1 - f_m^1\|_P < \frac{\epsilon}{2},$$

which implies that

$$\|f_n^0 - f_m^0\|_P \leq \|f_n^1 - f_m^1\|_P + \|f_n - f_m\|_P < \epsilon,$$

so  $\{f_n^0\}$  is also Cauchy with respect to  $\|\cdot\|_P$ . Since  $\mathcal{H}^0$  is finite dimensional and  $\langle \cdot, \cdot \rangle_P$  induces a (strict) norm on  $\mathcal{H}^0$ ,  $\mathcal{H}^0$  is complete with respect to  $\|\cdot\|_P$ , so there exists  $f^{*0} \in \mathcal{H}^0$  such that

$$\|f_n^0 - f^{*0}\|_P \longrightarrow 0. \quad (68)$$

Finally, let  $f^* = f^{*0} + f^{*1}$ , we have  $f^* \in \mathcal{H}$ . Combining (66), (67) and (68), we see that

$$\begin{aligned} \|f_n - f^*\|_*^2 &= \|f_n - f^*\|_P^2 + \alpha \|f_n - f^*\|_{k^1}^2 \\ &\leq 2\|f_n^0 - f^{*0}\|_P^2 + 2\|f_n^1 - f^{*1}\|_P^2 + \alpha \|f_n^1 - f^{*1}\|_{k^1}^2 \longrightarrow 0. \end{aligned}$$

Since every Cauchy sequence converges in  $(\mathcal{H}, \langle \cdot, \cdot \rangle_*)$ , we see that  $\mathcal{H}$  is a Hilbert space with respect to the inner product  $\langle \cdot, \cdot \rangle_*$ .

To check the reproducing property of  $\mathcal{H}$  with respect to  $\langle \cdot, \cdot \rangle_*$ , we need to show that the evaluation functionals  $\delta_x(f) = f(x)$  are bounded for all  $x \in \mathcal{X}$ . Suppose  $f = f^0 + f^1, f^0 \in \mathcal{H}^0, f^1 \in \mathcal{H}^1$ . Under Assumption 1,

$$|f^1(x)| = |\langle f^1, k_x^1 \rangle_{k^1}| \leq \|k_x^1\|_{k^1} \|f^1\|_{k^1} \leq \sqrt{k^1(x, x)} \frac{1}{\sqrt{\alpha}} \|f\|_* \leq M \|f\|_*, \quad (69)$$

where  $M = \sup_{x \in \mathcal{X}} \sqrt{k^1(x, x)} \frac{1}{\sqrt{\alpha}} < \infty$ . On the other hand, since  $\langle \cdot, \cdot \rangle_{k^0} := \langle \cdot, \cdot \rangle_P$  and  $\|f^1\|_P \leq 2\|f^1\|_\infty \leq 2M\|f\|_\star$ , we have

$$\begin{aligned} |f^0(x)| &= |\langle f^0, k_x^0 \rangle_{k^0}| \leq \|k_x^0\|_{k^0} \|f^0\|_{k^0} = \|k_x^0\|_P \|f^0\|_P \\ &\leq \|k_x^0\|_P (\|f\|_P + \|f^1\|_P) \leq \|k_x^0\|_P (\|f\|_\star + 2M\|f\|_\star) = d_x \|f\|_\star \end{aligned}$$

where  $d_x = \|k_x^0\|_P(2M + 1)$ . So  $|f(x)| \leq |f^0(x)| + |f^1(x)| \leq C_x \|f\|_\star$  for some constant  $C_x < \infty$  for all  $x \in \mathcal{X}$ . This then implies that  $\mathcal{H}$  is an RKHS with respect to  $\langle \cdot, \cdot \rangle_\star$ .  $\square$

## Proof of Theorem 4

*Proof.* Throughout, it is understood that  $\mathcal{H}_j \subset L^2(\mathcal{X}_j, dP_j)$  is endowed with  $\langle \cdot, \cdot \rangle_{\star_j}$ , for  $1 \leq j \leq p$ . To see that  $\mathbf{S}_{ij}$  is well-defined, we need to show the existence and uniqueness of the solution of the “generalized” regularized population regression problem. First, note that given  $\phi_j \in \mathcal{H}_j$ , the operator  $\text{Cov}[\phi_j(X_j), \cdot(X_i)] : \mathcal{H}_i \rightarrow \mathbb{R}$  is a bounded linear functional on  $\mathcal{H}_i$ . By the Riesz Representation Theorem, there exists a unique  $h \in \mathcal{H}_i$  such that  $\text{Cov}[\phi_j(X_j), f(X_i)] = \langle h, f \rangle_{\star_i}$  for all  $f \in \mathcal{H}_i$ . It then follows that

$$\begin{aligned} &\underset{f \in \mathcal{H}_i}{\text{argmin}} \left\{ \text{Var}[\phi_j(X_j) - f(X_i)] + \alpha_i \|f\|_{k_i^1}^2 \right\} \\ &= \underset{f \in \mathcal{H}_i}{\text{argmin}} \left\{ -2\text{Cov}[\phi_j(X_j), f(X_i)] + \text{Var}[f(X_i)] + \alpha_i \|f\|_{k_i^1}^2 \right\} \\ &= \underset{f \in \mathcal{H}_i}{\text{argmin}} \left\{ -2\langle h, f \rangle_{\star_i} + \|f\|_{\star_i}^2 \right\} \\ &= h. \end{aligned}$$

That is, we have  $\mathbf{S}_{ij}\phi_j = h$ , where  $h$  is unique and satisfies  $\text{Cov}[\phi_j(X_j), f(X_i)] = \langle h, f \rangle_{\star_i}$  for all  $f \in \mathcal{H}_i$ . Equivalently,

$$\text{Cov}[\phi_i(X_i), \phi_j(X_j)] = \langle \phi_i, \mathbf{S}_{ij}\phi_j \rangle_{\star_i}, \quad \forall \phi_i \in \mathcal{H}_i, \phi_j \in \mathcal{H}_j.$$

To check the properties of  $\mathbf{S}_{ij}$ , we first note that we can decompose the operation of  $\mathbf{S}_{ij}$  as follows:

$$\begin{array}{ccccccc} \mathbf{S}_{ij} : \mathcal{H}_j & \xrightarrow{\mathbf{I}} & L^2(\mathcal{X}_j, dP_j) & \xrightarrow{\mathbf{T}} & \mathcal{H}_i^* & \xrightarrow{\mathbf{R}} & \mathcal{H}_i, \\ \phi_j & \xmapsto{\mathbf{I}} & \phi_j & \xmapsto{\mathbf{T}} & \text{Cov}[\phi_j(X_j), \cdot(X_i)] & \xmapsto{\mathbf{R}} & h. \end{array}$$

Here  $\mathcal{H}_i^*$  denotes the dual space of  $\mathcal{H}_i$ , and consists of bounded linear functionals defined on  $\mathcal{H}_i$ . On the other hand,  $\mathbf{I} : \mathcal{H}_j \rightarrow L^2(\mathcal{X}_j, dP_j)$  denotes the inclusion of  $\mathcal{H}_j$  into  $L^2(\mathcal{X}_j, dP_j)$ ,  $\mathbf{T} : L^2(\mathcal{X}_j, dP_j) \rightarrow \mathcal{H}_i^*$  denotes the one-to-one correspondence between the function  $\phi_j \in L^2(\mathcal{X}_j, dP_j)$  (in fact, its corresponding equivalence class with respect to the squared-norm  $\text{Var}[\cdot(X_j)]$ ) and the bounded linear functional  $\text{Cov}[\phi_j(X_j), \cdot(X_i)] : \mathcal{H}_i \rightarrow \mathbb{R}$ , and  $\mathbf{R} : \mathcal{H}_i^* \rightarrow \mathcal{H}_i$  is the isomorphism between  $\text{Cov}[\phi_j(X_j), \cdot(X_i)] \in \mathcal{H}_i^*$  and the function  $h \in \mathcal{H}_i$ . Therefore, we have  $\mathbf{S}_{ij} = \mathbf{R}\mathbf{T}\mathbf{I}$ .

- **Linearity and boundedness:**

$\mathbf{S}_{ij} : \mathcal{H}_j \rightarrow \mathcal{H}_i$  is a bounded linear operator as long as each of  $\mathbf{R}, \mathbf{T}, \mathbf{I}$  is. That  $\mathbf{R}$  and  $\mathbf{I}$  are bounded and linear follows immediately. To check the linearity of  $\mathbf{T}$ , for all  $f \in \mathcal{H}_i$  and  $a, b \in \mathbb{R}$ , we have

$$\begin{aligned} \mathbf{T}(a\phi_j + b\psi_j)(f) &= \text{Cov}[a\phi_j(X_j) + b\psi_j(X_j), f(X_i)] \\ &= a\text{Cov}[\phi_j(X_j), f(X_i)] + b\text{Cov}[\psi_j(X_j), f(X_i)] \\ &= a\mathbf{T}(\phi_j)(f) + b\mathbf{T}(\psi_j)(f), \end{aligned}$$

so linearity follows. We now check that  $\mathbf{T}$  is bounded with operator norm less than or equal to one.

$$\begin{aligned}
\|\mathbf{T}\| &= \sup_{\phi_j: \text{Var}[\phi_j(X_j)] \leq 1} \|\mathbf{T}(\phi_j)\| \\
&= \sup_{\phi_j: \text{Var}[\phi_j(X_j)] \leq 1} \sup_{f: \|f\|_{\star_i} \leq 1} |\text{Cov}[\phi_j(X_j), f(X_i)]| \\
&\leq \sup_{\phi_j: \text{Var}[\phi_j(X_j)] \leq 1} \sup_{f: \|f\|_{\star_i} \leq 1} (\text{Var}[\phi_j(X_j)] \text{Var}[f(X_i)])^{1/2} \\
&\leq \sup_{\phi_j: \text{Var}[\phi_j(X_j)] \leq 1} \sup_{f: \|f\|_{\star_i} \leq 1} (\text{Var}[\phi_j(X_j)])^{1/2} \|f\|_{\star_i} \\
&= 1.
\end{aligned}$$

In fact, in the case when  $i = j$ , the operator norm of  $\mathbf{T}$  is exactly equal to one provided  $\dim(\mathcal{H}_j^0) > 0$ , since we can pick  $\phi_j \in \mathcal{H}_j^0$  with  $\text{Var}[\phi_j(X_j)] = 1$ , in which case  $\|\phi_j\|_{\star_j} = (\text{Var}[\phi_j(X_j)])^{1/2} = 1$  and both inequalities above become equalities.

- **Compactness:**

Using the fact that the product of a bounded linear operator and a compact operator is compact (see, e.g. [Reed and Simon \(1980\)](#), Theorem VI.12(c)), it suffices to show that one of  $\mathbf{R}$ ,  $\mathbf{T}$  or  $\mathbf{I}$  is compact. We are off to show the compactness of  $\mathbf{I}$ , which requires that every bounded sequence  $\{f_n\}$  in  $(\mathcal{H}_j, \langle \cdot, \cdot \rangle_{\star_j})$  has a convergent subsequence in  $L^2(\mathcal{X}_j, dP_j)$  (endowed with squared-norm  $\text{Var}[\cdot(X_j)]$ ).

To simplify notation, we omit the subscript  $j$ . Also, we define the semi-norm

$$\langle f, g \rangle_P := \text{Cov}[f(X), g(X)], \quad f, g \in L^2(\mathcal{X}, dP),$$

where  $X$  is a random variable taking values in  $\mathcal{X}$  with probability distribution  $P$ .

This proof idea is to establish that  $\{f_n\} \subset \mathcal{H}$  is uniformly bounded and equicontinuous and then invoke the Arzelà-Ascoli Theorem. We first recall that  $\mathcal{H}$  is also an RKHS with respect to  $\langle \cdot, \cdot \rangle_k$ . If  $\|f_n\|_{\star} \leq B$ , then by definition we have

$$\|f_n^1\|_{k^1} \leq \frac{\|f_n\|_{\star}}{\sqrt{\alpha}} \leq \frac{B}{\sqrt{\alpha}}$$

and

$$\begin{aligned}
\|f_n^0\|_{k^0} &= \|f_n^0\|_P \leq \|f_n^1\|_P + \|f_n\|_P \leq 2\|f_n^1\|_{\infty} + \|f_n\|_{\star} \\
&\leq 2M\|f_n\|_{\star} + \|f_n\|_{\star} \leq (2M+1)B,
\end{aligned}$$

where the second to the last inequality follows from (69). So

$$\|f_n\|_k = \|f_n^0 + f_n^1\|_k \leq \|f_n^0\|_{k^0} + \|f_n^1\|_{k^1} \leq C,$$

where  $C = (2M+1)B + B/\sqrt{\alpha} < \infty$ .

Under Assumption 1,  $k$  is uniformly continuous on  $\mathcal{X} \times \mathcal{X}$  and  $\sup_{x \in \mathcal{X}} k(x, x) < \infty$ . Since

$$|f_n(x)| = |\langle f_n, k_x \rangle_k| \leq \|f_n\|_k \|k_x\|_k = \|f_n\|_k \sqrt{k(x, x)},$$

and

$$\|f_n\|_\infty \leq \|f_n\|_k \sqrt{\sup_{x \in \mathcal{X}} k(x, x)} \leq C \sqrt{\sup_{x \in \mathcal{X}} k(x, x)} < \infty,$$

$\{f_n\}$  is uniformly bounded. To check that  $\{f_n\}$  is equicontinuous, note that

$$|f_n(x) - f_n(x')| = |\langle f_n, k_x - k_{x'} \rangle_k| \leq \|f_n\|_k \|k_x - k_{x'}\|_k \leq C \|k_x - k_{x'}\|_k, \quad (70)$$

and

$$\begin{aligned} \|k_x - k_{x'}\|_k^2 &= \langle k_x - k_{x'}, k_x - k_{x'} \rangle_k = k(x, x) - 2k(x, x') + k(x', x') \\ &\leq 2 \sup_{z \in \mathcal{X}} |k(z, x) - k(z, x')|. \end{aligned} \quad (71)$$

It then follows from (70), (71) and the uniform continuity of  $k$  on  $\mathcal{X} \times \mathcal{X}$  that  $\{f_n\}$  is equicontinuous. Applying the Arzelà-Ascoli Theorem,  $\{f_n\}$  contains a uniformly convergent subsequence  $\{f_{n_k}\}$ . Since  $\|f_{n_k}\|_P \leq 2\|f_{n_k}\|_\infty$ , it follows that  $\{f_{n_k}\}$  also converges in  $L^2(\mathcal{X}, dP)$ . So the inclusion  $\mathbf{I} : \mathcal{H} \hookrightarrow L^2(\mathcal{X}, dP)$  is compact.

To show (31), recall that Riesz Representation Theorem tells us that if  $\ell$  is a bounded linear functional on  $\mathcal{H}$  with representer  $h_\ell \in \mathcal{H}$ , i.e.  $\ell(f) = \langle h_\ell, f \rangle_\star$  for all  $f \in \mathcal{H}$ , then  $\|\ell\| = \|h_\ell\|_\star$ . In the case where  $\ell(f) = \text{Cov}[\phi_j(X_j), f(X_i)] = \langle h, f \rangle_{\star_i}$  for all  $f \in \mathcal{H}_i$ , we have

$$\begin{aligned} \|\mathbf{S}_{ij}\phi_j\|_{\star_i} &= \|h\|_{\star_i} = \|\text{Cov}[\phi_j(X_j), \cdot(X_i)]\| = \sup_{\|f\|_{\star_i} \leq 1} |\text{Cov}[\phi_j(X_j), f(X_i)]| \\ &\leq \sup_{\|f\|_{\star_i} \leq 1} (\text{Var}[\phi_j(X_j)] \text{Var}[f(X_i)])^{1/2} \\ &\leq \sup_{\|f\|_{\star_i} \leq 1} (\text{Var}[\phi_j(X_j)])^{1/2} \|f\|_{\star_i} = (\text{Var}[\phi_j(X_j)])^{1/2} \leq \|\phi_j\|_{\star_j}. \end{aligned}$$

□

## Proof of Theorem 5

*Proof.* First, note that we can rewrite the optimization criterion in the kernelized population APC problem as

$$\begin{aligned} &\text{Var} \left[ \sum_i \phi_i(X_i) \right] + \sum_i \alpha_i \|\phi_i\|_{k_i^1}^2 \\ &= \sum_i \text{Var}[\phi_i(X_i)] + \sum_i \alpha_i \|\phi_i\|_{k_i^1}^2 + \sum_i \sum_{j \neq i} \text{Cov}[\phi_i(X_i), \phi_j(X_j)] \\ &= \sum_i \|\phi_i\|_{\star_i}^2 + \sum_i \sum_{j \neq i} \langle \phi_i, \mathbf{S}_{ij}\phi_j \rangle_{\star_i} \\ &= \sum_i \left\langle \phi_i, \sum_{j \neq i} \mathbf{S}_{ij}\phi_j + \phi_i \right\rangle_{\star_i} \\ &= \langle \Phi, \tilde{\mathbf{S}}\Phi \rangle_\star \geq 0. \end{aligned}$$

Hence,  $\tilde{\mathbf{S}}$  is positive. That the constraint  $\sum \text{Var} \phi_i(X_i) + \sum \alpha_i \|\phi_i\|_{k_i^1}^2 = \langle \Phi, \Phi \rangle_\star$  follows by definition.

To see that  $\tilde{\mathbf{S}}$  is self-adjoint, we need to show that  $\langle \Phi, \tilde{\mathbf{S}}\Psi \rangle_\star = \langle \tilde{\mathbf{S}}\Phi, \Psi \rangle_\star$ . Since

$$\text{Cov}[\phi_i(X_i), \psi_j(X_j)] = \langle \phi_i, \mathbf{S}_{ij}\psi_j \rangle_{\star_i} = \langle \mathbf{S}_{ji}\phi_i, \psi_j \rangle_{\star_j}, \quad \forall \phi_i \in \mathcal{H}_i, \psi_j \in \mathcal{H}_j,$$

giving  $\mathbf{S}_{ij}^* = \mathbf{S}_{ji}$ , we have

$$\begin{aligned}
\langle \Phi, \tilde{\mathbf{S}} \Psi \rangle_{\star} &= \sum_i \langle \phi_i, [\tilde{\mathbf{S}} \Psi]_i \rangle_{\star_i} = \sum_i \left\langle \phi_i, \sum_{j \neq i} \mathbf{S}_{ij} \psi_j + \psi_i \right\rangle_{\star_i} \\
&= \sum_i \sum_{j \neq i} \langle \phi_i, \mathbf{S}_{ij} \psi_j \rangle_{\star_i} + \sum_i \langle \phi_i, \psi_i \rangle_{\star_i} = \sum_j \sum_{i \neq j} \langle \mathbf{S}_{ji} \phi_i, \psi_j \rangle_{\star_j} + \sum_j \langle \phi_j, \psi_j \rangle_{\star_j} \\
&= \sum_j \left\langle \sum_{i \neq j} \mathbf{S}_{ji} \phi_i + \phi_j, \psi_j \right\rangle_{\star_j} = \sum_j \langle [\tilde{\mathbf{S}} \Phi]_j, \psi_j \rangle_{\star_j} = \langle \tilde{\mathbf{S}} \Phi, \Psi \rangle_{\star},
\end{aligned}$$

and so  $\tilde{\mathbf{S}}$  is self-adjoint.

To check that  $\tilde{\mathbf{S}}$  is bounded above by  $p$ , by (31), we have  $\|\mathbf{S}_{ij} \phi_j\|_{\star_i} \leq \|\phi_j\|_{\star_j}$ . Therefore,

$$\begin{aligned}
\|\tilde{\mathbf{S}} \Phi\|_{\star}^2 &= \sum_{i=1}^p \left\| \sum_{j \neq i} \mathbf{S}_{ij} \phi_j + \phi_i \right\|_{\star_i}^2 \leq \sum_{i=1}^p \left( \sum_{j \neq i} \|\mathbf{S}_{ij} \phi_j\|_{\star_i} + \|\phi_i\|_{\star_i} \right)^2 \\
&\leq \sum_{i=1}^p \left( \sum_{j=1}^p \|\phi_j\|_{\star_j} \right)^2 \quad \text{since } \|\mathbf{S}_{ij} \phi_j\|_{\star_i} \leq \|\phi_j\|_{\star_j} \\
&\leq p \cdot p \sum_{j=1}^p \|\phi_j\|_{\star_j}^2 \quad \text{since } \left( \sum_{j=1}^p a_j \right)^2 \leq p \sum_{j=1}^p a_j^2 \text{ if } a_j \geq 0 \text{ for } 1 \leq j \leq p \\
&= p^2 \|\Phi\|_{\star}^2,
\end{aligned}$$

so  $\|\tilde{\mathbf{S}}\| = \sup_{\|\Phi\|_{\star} \leq 1} \|\tilde{\mathbf{S}} \Phi\|_{\star} \leq p$ . □

### Proof of Theorem 6

*Proof.* We can decompose  $\tilde{\mathbf{S}} - \mathbf{I}$  as  $\tilde{\mathbf{S}} - \mathbf{I} = \sum_{j=1}^p \mathbf{T}_j$ , where  $\mathbf{T}_j : \mathcal{H} \rightarrow \mathcal{H}$  is defined by

$$\mathbf{T}_j(\Phi) = (\mathbf{S}_{1j}(\phi_j), \dots, \mathbf{S}_{j-1,j}(\phi_j), \mathbf{0}, \mathbf{S}_{j+1,j}(\phi_j), \dots, \mathbf{S}_{pj}(\phi_j)).$$

It is sufficient to show that every summand  $\mathbf{T}_j$  is compact. Let  $\mathbf{B}$  be the unit ball in  $\mathcal{H}$ , our goal is then to show that  $\mathbf{T}_j(\mathbf{B})$  is a relatively compact set in  $\mathcal{H}$ . Let  $B_j$  be the unit ball in  $\mathcal{H}_j$ , then since  $\mathbf{B} \subset B_1 \times \dots \times B_p$ , compactness of  $\mathbf{T}_j$  follows if  $\mathbf{T}_j(B_1 \times \dots \times B_p)$  is shown to be relatively compact. By Theorem 4,  $\mathbf{S}_{ij}(B_j)$  is relatively compact in  $\mathcal{H}_j$ , so

$$\mathbf{T}_j(B_1 \times \dots \times B_p) = \mathbf{S}_{1j}(B_j) \times \dots \times \mathbf{S}_{j-1,j}(B_j) \times \{0\} \times \mathbf{S}_{j+1,j}(B_j) \times \dots \times \mathbf{S}_{pj}(B_j)$$

is relatively compact in  $\mathcal{H}$ , since the norm topology and the product topology coincide. □

### Proof of Proposition 1

*Proof.* Let  $\mathbf{M} = \gamma \mathbf{I} - \tilde{\mathbf{S}}$ , where  $\gamma = (p+1)/2$ . Then  $\tilde{\Phi}$  is the unit eigenfunction corresponding to the largest eigenvalue  $\lambda$  of  $\mathbf{M}$ , and it is assumed that  $\lambda$  has multiplicity one. By assumption, the power algorithm is initialized with  $\Phi^{[0]}$  that satisfies

$$\Phi^{[0]} = a_0 \tilde{\Phi} + \Psi^{[0]}, \quad \text{where } \Psi^{[0]} \perp \tilde{\Phi} \text{ and } a_0 > 0.$$

Let

$$\Phi^{[t+1]} = \frac{\mathbf{M} \Phi^{[t]}}{\|\mathbf{M} \Phi^{[t]}\|_{\star}},$$



and suppose that

$$\Phi^{[t]} = a_t \tilde{\Phi} + \Psi^{[t]}, \quad \text{where } \Psi^{[t]} \perp \tilde{\Phi}.$$

Then

$$\Phi^{[t+1]} = \frac{\mathbf{M}\Phi^{[t]}}{\|\mathbf{M}\Phi^{[t]}\|_*} = \frac{\mathbf{M}(a_t \tilde{\Phi} + \Psi^{[t]})}{\|\mathbf{M}\Phi^{[t]}\|_*} = \frac{a_t \lambda}{\|\mathbf{M}\Phi^{[t]}\|_*} \tilde{\Phi} + \frac{\mathbf{M}\Psi^{[t]}}{\|\mathbf{M}\Phi^{[t]}\|_*}.$$

Matching the coefficients, we see that

$$a_{t+1} = \frac{a_t \lambda}{\|\mathbf{M}\Phi^{[t]}\|_*}, \quad \Psi^{[t+1]} = \frac{\mathbf{M}\Psi^{[t]}}{\|\mathbf{M}\Phi^{[t]}\|_*}, \quad (72)$$

and it follows that  $a_0 > 0$  implies  $a_t > 0$  for all  $t \in \mathbb{N}$ . Now note that for  $\Psi \perp \tilde{\Phi}$ ,

$$\|\mathbf{M}\Psi\|_* \leq r \|\Psi\|_*, \quad \text{where } r < \lambda, \quad (73)$$

so by (72) and (73),

$$\frac{\|\Psi^{[t+1]}\|_*}{a_{t+1}} = \frac{\|\mathbf{M}\Psi^{[t]}\|_*}{a_t \lambda} \leq \left(\frac{r}{\lambda}\right) \frac{\|\Psi^{[t]}\|_*}{a_t},$$

which in turn implies

$$\frac{\|\Psi^{[t]}\|_*}{a_t} \leq \left(\frac{r}{\lambda}\right)^t \frac{\|\Psi^{[0]}\|_*}{a_0} \rightarrow 0 \text{ as } t \rightarrow \infty. \quad (74)$$

To show that  $\Phi^{[t]} \rightarrow \tilde{\Phi}$ , note that  $\|\Phi^{[t]}\| = 1$  implies that

$$\|a_t \tilde{\Phi} + \Psi^{[t]}\|_* = 1 \iff a_t^2 + \|\Psi^{[t]}\|_*^2 = 1 \iff 1 + \frac{\|\Psi^{[t]}\|_*^2}{a_t^2} = \frac{1}{a_t^2}.$$

By (74) we have  $a_t^2 \rightarrow 1$  and  $\|\Psi^{[t]}\|_*^2 \rightarrow 0$ , hence

$$\|\Phi^{[t]} - \tilde{\Phi}\|_*^2 = (1 - a_t)^2 + \|\Psi^{[t]}\|_*^2 \rightarrow 0.$$

□

## C Implementation Details of the Power Algorithm

We justified the use of a smoothing-based power algorithm in computing kernelized population APCs in Section 7. In this section, we give a detailed description of its empirical implementation.

We first need to resolve the issue that the function space  $\mathcal{H}$  in the kernelized sample APC problem (16) are (almost always) infinite-dimensional, which can pose challenges computationally. As will be shown, the solution to (16) always lie in a finite-dimensional subspace of  $\mathcal{H}$ . Consider the smoothing splines problem

$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \alpha \|f\|_{k^1}^2 \right\}, \quad (75)$$

where  $\mathcal{H} = \mathcal{H}^0 \oplus \mathcal{H}^1$ ,  $\dim(\mathcal{H}^0) = m < n$ , and  $\mathcal{H}^1$  is an RKHS with reproducing kernel  $k^1$ . It is known that the solution  $\hat{f}$  of (75) must lie in a finite-dimensional subspace of  $\mathcal{H}$ . Specifically, write  $\hat{f} = \hat{f}^0 + \hat{f}^1$  with  $\hat{f}^0 \in \mathcal{H}^0$ ,  $\hat{f}^1 \in \mathcal{H}^1$ , then

$$\hat{f}^1 \in \text{span}\{k^1(x_i, \cdot) : 1 \leq i \leq n\}.$$

In essence, this means that to solve (75), only the representers of the evaluation functionals (projected to  $\mathcal{H}^1$ ) at the locations of the observed data matters. This is known as the *Representer Theorem for smoothing splines*. A more general version of this Representer Theorem, adapted to the case of kernelized APCs, states that for any probability measure  $P_j(dx_j)$ , not necessarily an empirical measure, only the representers of the evaluation functionals at the locations that belong to the support of  $P_j$  matters.

**Theorem 7** (Representer Theorem for Kernelized APCs). *The solution to the kernelized APC problem (13), if exists, is taken on the subspace  $\mathcal{H}_P := \mathcal{H}_{P_1} \times \mathcal{H}_{P_2} \times \cdots \times \mathcal{H}_{P_p}$ , where*

$$\mathcal{H}_{P_j} := \mathcal{H}_j^0 \oplus \overline{\text{span}\{k_j^1(x, \cdot) - m_j^1 : x \in \text{supp}(P_j)\}},$$

and  $m_j^1$  is the mean element of  $\mathcal{H}_j^1$  with respect to  $P_j$ .

*Proof.* Let  $m_j = m_j^0 + m_j^1$  be the mean element of  $\mathcal{H}_j$  with respect to  $P_j$ , where  $m_j^0 \in \mathcal{H}_j^0$  and  $m_j^1 \in \mathcal{H}_j^1$ . For  $\psi_j \in \mathcal{H}_j$ , we have

$$\psi_j \perp \mathcal{H}_{P_j} \Rightarrow \psi_j(x) - E\psi_j = 0, \quad \text{for } x \in \text{supp}(P_j).$$

This is because  $\psi_j(x) - E\psi_j = \langle \psi_j, k_j(x, \cdot) - m_j \rangle_{k_j} = \langle \psi_j, k_j^0(x, \cdot) - m_j^0 \rangle_{k_j} + \langle \psi_j, k_j^1(x, \cdot) - m_j^1 \rangle_{k_j}$  and  $k_j^0(x, \cdot) - m_j^0 \in \mathcal{H}_j^0$ . So given  $\psi_j \perp \mathcal{H}_{P_j}$  and  $\phi_j \in \mathcal{H}_{P_j}$ , we have  $\text{Var } \psi_j = 0$  and  $\|\phi_j + \psi_j\|_{k_j^1}^2 = \|\phi_j\|_{k_j^1}^2 + \|\psi_j\|_{k_j^1}^2$ , which implies that

$$\text{Var } \sum_{j=1}^p (\phi_j + \psi_j) = \text{Var } \sum_{j=1}^p \phi_j, \quad \sum_{j=1}^p \alpha_j \|\phi_j + \psi_j\|_{k_j^1}^2 \geq \sum_{j=1}^p \alpha_j \|\phi_j\|_{k_j^1}^2,$$

and the inequality is strict when  $\psi_i \neq 0$  for some  $1 \leq i \leq p$ .

Now, suppose on the contrary that  $(\phi_1^* + \psi_1^*, \dots, \phi_p^* + \psi_p^*)$  is the optimal solution of the kernelized APC problem, where  $\phi_j^* \in \mathcal{H}_{P_j}$ ,  $\psi_j^* \perp \mathcal{H}_{P_j}$  and  $\psi_i^* \neq 0$  for some  $1 \leq i \leq p$ . Let

$$\delta = \sum_{j=1}^p \alpha_j \|\phi_j^* + \psi_j^*\|_{k_j^1}^2,$$

then  $(\phi_1^* + \psi_1^*, \dots, \phi_p^* + \psi_p^*)$  is also an optimal solution of the following optimization problem:

$$\min_{\Phi \in \mathcal{H}} \text{Var } \sum_{j=1}^p \phi_j + \sum_{j=1}^p \alpha_j \|\phi_j\|_{k_j^1}^2 \quad \text{subject to} \quad \sum_{j=1}^p \text{Var } \phi_j = 1 - \delta. \quad (76)$$

But as argued before we have  $\text{Var } \sum (\phi_j^* + \psi_j^*) = \text{Var } (\sum \phi_j^*)$  and  $\sum \alpha_j \|\phi_j^* + \psi_j^*\|_{k_j^1}^2 > \sum \alpha_j \|\phi_j^*\|_{k_j^1}^2$ . Also, subject to the constraint that  $\sum \text{Var } (\phi_j^* + \psi_j^*) = 1 - \delta$ , we have  $\sum \text{Var } \phi_j^* = 1 - \delta$ . This gives the desired contradiction since in this case  $(\phi_1^*, \dots, \phi_p^*)$  is a better solution of (76) comparing to the optimal solution  $(\phi_1^* + \psi_1^*, \dots, \phi_p^* + \psi_p^*)$ . Therefore, we must have  $\psi_j^* \equiv 0$  for  $1 \leq j \leq p$ , and the proof is complete.  $\square$

Note that in the case where  $P_j$  denotes the empirical probability measure with only finitely many values  $\{x_{1j}, \dots, x_{n_j}\}$  in its support, Theorem 7 specializes to the finite-sample version of the Representer Theorem for kernelized APCs:

**Corollary 3.** *Given data  $\mathbf{x}_i = (x_{i1}, \dots, x_{ip})$ ,  $1 \leq i \leq n$ , the solution of the kernelized sample APC problem (16), if exists, is taken on the finite-dimensional subspace  $\mathcal{H}_n := \mathcal{H}_{n,1} \times \dots \times \mathcal{H}_{n,p}$ , where*

$$\mathcal{H}_{n,j} := \mathcal{H}_j^0 \oplus \text{span} \left\{ k_j^1(x_{ij}, \cdot) - \frac{1}{n} \sum_{a=1}^n k_j^1(x_{aj}, \cdot) : 1 \leq i \leq n \right\}.$$

One can similarly show that other higher-order kernelized sample APCs, if exists, also lie in the finite-dimensional subspace  $\mathcal{H}_n$ .

To implement the power algorithm, it follows from Corollary 3 that it suffices to work with the coefficients of the basis of  $\mathcal{H}_{n,i}$ . Specifically, let  $\phi_i = \sum_{\ell=1}^n \beta_{\ell i} f_{\ell i} + \sum_{\ell=1}^{m_i} \beta_{n+\ell,i} q_{\ell i}$ , where  $f_{\ell i} = k_i^1(x_{\ell i}, \cdot) - \frac{1}{n} \sum_{a=1}^n k_i^1(x_{ai}, \cdot)$ ,  $1 \leq \ell \leq n$ . Then the update steps  $\phi_i \leftarrow \gamma \phi_i^{[t]} - (\sum_{j \neq i} \mathbf{S}_{ij} \phi_j^{[t]} + \phi_i^{[t]})$  in Algorithm 1 becomes

$$\begin{aligned} \beta_{\ell i} &\leftarrow (\gamma - 1) \beta_{\ell i}^{[t]} - c_{\ell i}, & 1 \leq \ell \leq n, \\ \beta_{n+\ell,i} &\leftarrow (\gamma - 1) \beta_{n+\ell,i}^{[t]} - d_{\ell i}, & 1 \leq \ell \leq m_i, \end{aligned} \quad (77)$$

where  $\{c_{\ell i}\}_{\ell=1}^n$  and  $\{d_{\ell i}\}_{\ell=1}^{m_i}$  are two sets of coefficients obtained from the smoothing step  $\sum_{j \neq i} \mathbf{S}_{ij} \phi_j^{[t]}$ , which will be derived shortly.

Let  $\boldsymbol{\beta}_i = (\beta_{1i}, \dots, \beta_{ni})$ , and let  $\mathbf{G}_i$  be the  $n \times n$  centered Gram matrix associated with  $k_i^1$ , with  $(j, \ell)$  entry

$$\begin{aligned} (\mathbf{G}_i)_{j\ell} &= \langle f_{ji}, f_{\ell i} \rangle_{k_i^1} \\ &= k_i^1(x_{ji}, x_{\ell i}) - \frac{1}{n} \sum_{b=1}^n k_i^1(x_{ji}, x_{bi}) - \frac{1}{n} \sum_{a=1}^n k_i^1(x_{ai}, x_{\ell i}) + \frac{1}{n^2} \sum_{a=1}^n \sum_{b=1}^n k_i^1(x_{ai}, x_{bi}). \end{aligned} \quad (78)$$

Then the normalizing constant  $c$  in Algorithm 1 can be obtained upon computation of the variance of the transformed data points  $\{\phi_i(x_{\ell i})\}_{\ell=1}^n$  and the penalty term  $\|\phi_i\|_{k_i^1}^2 = \boldsymbol{\beta}_i^T \mathbf{G}_i \boldsymbol{\beta}_i$ , for  $1 \leq i \leq p$ .

We now consider the smoothing step  $\sum_{j \neq i} \mathbf{S}_{ij} \phi_j$ , which by linearity of smoothing is empirically the regularized least squares regression of  $\sum_{j \neq i} \phi_j$  against  $X_i$ . This amounts to solving the following optimization problem:

$$\min_{f \in \mathcal{H}_i} \left\{ \widehat{\text{Var}} \left[ \sum_{j \neq i} \phi_j(X_j) - f(X_i) \right] + \alpha_i \|f\|_{k_i^1}^2 \right\}, \quad (79)$$

where  $\widehat{\text{Var}} [\sum_{j \neq i} \phi_j(X_j) - f(X_i)]$  evaluates to

$$\frac{1}{n} \sum_{\ell=1}^n \left[ \sum_{j \neq i} \left( \phi_j(x_{\ell j}) - \frac{1}{n} \sum_{b=1}^n \phi_j(x_{bj}) \right) - \left( f(x_{\ell i}) - \frac{1}{n} \sum_{a=1}^n f(x_{ai}) \right) \right]^2.$$

We see that (79) is essentially the smoothing splines problem (75) (modulo centering), hence it is not surprising that its solution lies in  $\mathcal{H}_{n,i}$  as well.

Following Wahba (1990) (page 11-12), let the closed form solution of (79) be

$$f = \sum_{\ell=1}^n c_{\ell i} f_{\ell i} + \sum_{\ell=1}^{m_i} d_{\ell i} q_{\ell i},$$

and (79) can be restated as

$$\min_{\mathbf{c} \in \mathbb{R}^n, \mathbf{d} \in \mathbb{R}^{m_i}} \left\{ \frac{1}{n} \|\mathbf{y} - (\mathbf{G}_i \mathbf{c} + \mathbf{Q}_i \mathbf{d})\|^2 + \alpha_i \mathbf{c}^T \mathbf{G}_i \mathbf{c} \right\}, \quad (80)$$

where  $\mathbf{c}^T = (c_{1i}, \dots, c_{ni})$ ,  $\mathbf{d}^T = (d_{1i}, \dots, d_{m_i i})$ ,  $\mathbf{y}^T = (y_1, \dots, y_n)$  with  $y_\ell = \sum_{j \neq i} [\phi_j(x_{\ell j}) - \frac{1}{n} \sum_{b=1}^n \phi_j(x_{bj})]$  for  $1 \leq \ell \leq n$ ,  $\mathbf{G}_i$  is as given in (78), and  $\mathbf{Q}_i$  is the column-centered version of

$$\tilde{\mathbf{Q}}_i = \begin{pmatrix} q_{1i}(x_{1i}) & \cdots & q_{m_i i}(x_{1i}) \\ \vdots & \vdots & \vdots \\ q_{1i}(x_{ni}) & \cdots & q_{m_i i}(x_{ni}) \end{pmatrix}.$$

It then follows that the solution of (80) is

$$\mathbf{d} = (\mathbf{Q}_i^T \mathbf{M}_i^{-1} \mathbf{Q}_i)^{-1} \mathbf{Q}_i^T \mathbf{M}_i^{-1} \mathbf{y}, \quad \mathbf{c} = \mathbf{M}_i^{-1} (\mathbf{y} - \mathbf{Q}_i \mathbf{d}),$$

where  $\mathbf{M}_i = \mathbf{G}_i + n\alpha_i \mathbf{I}$ ,  $\mathbf{I}$  being the  $n \times n$  identity matrix. Plugging  $\mathbf{c}$  and  $\mathbf{d}$  into (77) completes the update steps.

## D A Direct Approach for Computing APCs

In this section, we give a direct approach for computing APCs.

From Corollary 3, we know that the solution  $\hat{\Phi} = (\hat{\phi}_1, \dots, \hat{\phi}_p)$  of the kernelized sample APC problem (16) lies in the finite-dimensional function space  $\mathcal{H}_n = \mathcal{H}_{n,1} \times \cdots \times \mathcal{H}_{n,p}$ . In the following, we derive the resulting linear algebra problem in terms of the coefficients with respect to the basis of  $\mathcal{H}_{n,j}$ 's. We will focus on the case where there are no null spaces, i.e.  $\mathcal{H}_j = \mathcal{H}_j^1$  and  $k_j = k_j^1$ , for  $1 \leq j \leq p$ . The case with null spaces requires the use of the additional basis  $\{q_{1j}, \dots, q_{m_j j}\}$  for  $\mathcal{H}_j^0$ ,  $1 \leq j \leq p$ , which is tractable but with slightly more tedious derivation. We recommend the use of power algorithm described in Section 7 when dealing with cases involving null spaces. The power algorithm is computationally more attractive than the direct linear algebra approach given below, when the interest is only in extracting a few eigenfunctions.

For each  $1 \leq j \leq p$ , we express  $\phi_j \in \mathcal{H}_{n,j}$  as  $\phi_j = \sum_{i=1}^n \beta_{ij} f_{ij}$ , where

$$f_{ij}(\cdot) := k_j^1(x_{ij}, \cdot) - \frac{1}{n} \sum_{a=1}^n k_j^1(x_{aj}, \cdot), \quad 1 \leq i \leq n.$$

Then

$$\begin{aligned} \sum_{j=1}^p \phi_j &= \sum_{j=1}^p \sum_{i=1}^n \beta_{ij} f_{ij} = \sum_{j=1}^p \beta_j^T \mathbf{f}_j \\ &\quad \text{where } \beta_j^T = (\beta_{1j}, \dots, \beta_{nj}), \mathbf{f}_j^T = (f_{1j}, \dots, f_{nj}) \\ &= \beta^T \mathbf{F} \quad \text{where } \beta^T = (\beta_1^T, \dots, \beta_p^T), \mathbf{F}^T = (\mathbf{f}_1^T, \dots, \mathbf{f}_p^T). \end{aligned}$$

The penalty term associated with  $\phi_j$  evaluates to

$$\|\phi_j\|_{k_j}^2 = \left\langle \sum_{i=1}^n \beta_{ij} f_{ij}, \sum_{\ell=1}^n \beta_{\ell j} f_{\ell j} \right\rangle_{k_j} = \sum_{i=1}^n \sum_{\ell=1}^n \beta_{ij} \beta_{\ell j} \langle f_{ij}, f_{\ell j} \rangle_{k_j} = \beta_j^T \mathbf{G}_j \beta_j,$$

where  $\mathbf{G}_j$  is the centered Gram matrix associated with  $k_j$ , with  $(i, \ell)$  entry

$$\begin{aligned} (\mathbf{G}_j)_{i\ell} &= \langle f_{ij}, f_{\ell j} \rangle_{k_j} \\ &= k_j(x_{ij}, x_{\ell j}) - \frac{1}{n} \sum_{b=1}^n k_j(x_{ij}, x_{bj}) - \frac{1}{n} \sum_{a=1}^n k_j(x_{aj}, x_{\ell j}) + \frac{1}{n^2} \sum_{a=1}^n \sum_{b=1}^n k_j(x_{aj}, x_{bj}). \end{aligned}$$

Therefore, we can rewrite the penalty term as

$$\sum_{j=1}^p \alpha_j \|\phi_j\|_{k_j}^2 = \sum_{j=1}^p \alpha_j \beta_j^T \mathbf{G}_j \beta_j.$$

The variance term in the criterion evaluates to

$$\widehat{\text{Var}} \sum_{j=1}^p \phi_j = \widehat{\text{Var}} (\beta^T \mathbf{F}) = \frac{1}{n} \beta^T \mathbf{G} \mathbf{G}^T \beta,$$

where  $\mathbf{G}^T = (\mathbf{G}_1, \dots, \mathbf{G}_p)$ . Meanwhile, the variance term in the constraint is

$$\sum_{j=1}^p \widehat{\text{Var}} \phi_j = \sum_{j=1}^p \widehat{\text{Var}} (\beta_j^T \mathbf{f}_j) = \frac{1}{n} \sum_{j=1}^p \beta_j^T \mathbf{G}_j^2 \beta_j.$$

Hence, the optimization problem (16), expressed in linear algebra notation, becomes

$$\begin{aligned} \min_{\beta \in \mathbb{R}^{pn}} \quad & \frac{1}{n} \beta^T \mathbf{G} \mathbf{G}^T \beta + \beta^T \text{diag}(\alpha_1 \mathbf{G}_1, \dots, \alpha_p \mathbf{G}_p) \beta \\ \text{subject to} \quad & \frac{1}{n} \beta^T \text{diag}(\mathbf{G}_1^2, \dots, \mathbf{G}_p^2) \beta + \beta^T \text{diag}(\alpha_1 \mathbf{G}_1, \dots, \alpha_p \mathbf{G}_p) \beta = 1. \end{aligned} \quad (81)$$

Equivalently, we want to solve the following generalized eigenvalue problem:

$$\begin{aligned} & \begin{pmatrix} \mathbf{G}_1^2 + n\alpha_1 \mathbf{G}_1 & \mathbf{G}_1 \mathbf{G}_2 & \cdots & \mathbf{G}_1 \mathbf{G}_p \\ \mathbf{G}_2 \mathbf{G}_1 & \mathbf{G}_2^2 + n\alpha_2 \mathbf{G}_2 & \cdots & \mathbf{G}_2 \mathbf{G}_p \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{G}_p \mathbf{G}_1 & \mathbf{G}_p \mathbf{G}_2 & \cdots & \mathbf{G}_p^2 + n\alpha_p \mathbf{G}_p \end{pmatrix} \beta \\ &= \lambda \begin{pmatrix} \mathbf{G}_1^2 + n\alpha_1 \mathbf{G}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{G}_2^2 + n\alpha_2 \mathbf{G}_2 & \ddots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{G}_p^2 + n\alpha_p \mathbf{G}_p \end{pmatrix} \beta. \end{aligned} \quad (82)$$

Following [Bach and Jordan \(2003\)](#), we can approximate the diagonal blocks  $\mathbf{G}_j^2 + n\alpha_j \mathbf{G}_j$  in (82) by  $(\mathbf{G}_j + \frac{n\alpha_j}{2} \mathbf{I})^2$ . Letting  $\gamma_j = (\mathbf{G}_j + \frac{n\alpha_j}{2} \mathbf{I}) \beta_j$  allows the reformulation of the generalized eigenproblem above as an eigenproblem, in which case we just need to perform eigendecomposition on

$$\mathbf{R} = \begin{pmatrix} \mathbf{I} & \mathbf{R}_1^T \mathbf{R}_2 & \cdots & \mathbf{R}_1^T \mathbf{R}_p \\ \mathbf{R}_2^T \mathbf{R}_1 & \mathbf{I} & \cdots & \mathbf{R}_2^T \mathbf{R}_p \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{R}_p^T \mathbf{R}_1 & \mathbf{R}_p^T \mathbf{R}_2 & \cdots & \mathbf{I} \end{pmatrix},$$

where  $\mathbf{R}_j = \mathbf{G}_j(\mathbf{G}_j + \frac{n\alpha_j}{2}\mathbf{I})^{-1}$  and  $\mathbf{I}$  is the  $n \times n$  identity matrix, to get its eigenvector  $\hat{\gamma} = (\hat{\gamma}_1, \dots, \hat{\gamma}_p)$  (corresponding to the smallest eigenvalue). The desired (approximate) solution of (81) can then be obtained as  $\hat{\beta}_j = (\mathbf{G}_j + \frac{n\alpha_j}{2}\mathbf{I})^{-1}\hat{\gamma}_j$ , while the (mean-centered) estimated transform evaluated at the data points is

$$\hat{\phi}_j = \mathbf{G}_j\hat{\beta}_j = \mathbf{G}_j\left(\mathbf{G}_j + \frac{n\alpha_j}{2}\mathbf{I}\right)^{-1}\hat{\gamma}_j.$$

The second smallest and subsequent higher order kernelized sample APCs can be obtained similarly by extracting the eigenvector corresponding to the second smallest and subsequent smallest eigenvalue of  $\mathbf{R}$ .

We remark that the linear algebra problem (81) is often numerically ill-conditioned due to low-rankness of  $\mathbf{G}_j$ , so one has to make adjustment in order to solve for APCs. This, however, introduces undesirable arbitrariness to the resulting optimization problem.